

# SETOL: A Semi-Empirical Theory of (Deep) Learning

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## Abstract

We present a Semi-Empirical Theory of Learning (**SETOL**) that explains the remarkable performance of State-of-the-Art (SOTA) Neural Networks (NNs). We provide a formal explanation of the origin of the fundamental quantities in the phenomenological theory of Heavy-Tailed Self-Regularization (**HTSR**), the Heavy-Tailed Power Law Layer Quality metrics, **AlphaHat** ( $\alpha$ ) and **AlphaHat** ( $\hat{\alpha}$ ). In prior work, these metrics have been shown to predict trends in the test accuracies of pretrained SOTA NN models, and, importantly, without needing access to the testing or even training data. Our **SETOL** uses techniques from Statistical Mechanics (**StatMech**) as well as advanced methods from Random Matrix Theory (**RMT**) and Quantum Chemistry. Our derivation suggests new mathematical preconditions for *Ideal* learning, including the new **ERG** metric (which is equivalent to applying a single step of the Wilson Exact Renormalization Group). We test the assumptions and predictions of our **SETOL** on a simple 3-layer Multi-Layer Perceptron (MLP), demonstrating excellent agreement with the key theoretical assumptions. For SOTA NN models, we show how to estimate the individual layer Qualities of a trained NN by simply computing the Empirical Spectral Density (ESD) of the layer weight matrices and then plugging this ESD into our **SETOL** formulae. Notably, we examine the performance of the **HTSR**  $\alpha$  and the **SETOL ERG** Layer Quality metrics, and find that they align remarkably well, both on our MLP and SOTA NNs.

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# 1 Introduction

Deep Neural Networks (DNNs)—models in the field of Artificial Intelligence (AI)—have driven remarkable advances in multiple fields of science and engineering. AlphaFold has made significant progress in solving the protein folding problem.[1] Notably, the 2024 Nobel Prize in Physics was awarded to Hopfield and Hinton for developing early approaches to AI using techniques from *Statistical Mechanics* (StatMech), and Jumper and Hassabis, along with Baker, received the 2024 Nobel Prize in Chemistry for their contributions to AlphaFold and computational protein design.[2, 3] Self-driving cars now roam the streets of major metropolitan cities like San Francisco. Large Language Models (LLMs) like ChatGPT have gained worldwide attention and initiated serious conversations about the possibility of creating an Artificial General Intelligence (AGI). Clearly, not a single area of science or engineering has ignored these remarkable advances in the field of AI and Neural Networks (NNs).

Despite this remarkable progress in a research field spanning over 50 years, developing, training, and maintaining such complex models require staggering capital resources, limiting their development to only the largest and best-funded organizations. While many such entities have open-sourced some of their largest models (such as Llama and Falcon), using these models requires assuming they have been trained optimally, without significant defects that could limit, skew, or even invalidate their use downstream. Moreover, testing such models can be very expensive and complex to interpret.

Because training and evaluating NNs is so hard, significant issues can manifest in many obvious and non-obvious ways. A primary research goal is to improve the efficiency and reduce the cost of training large NNs. A lesser-known but critical issue arises in many industrial settings, specifically “selecting the best models to test.” This arises in industries such as ad-click prediction, search relevance, quantitative trading, and more. Frequently, one has several seemingly equally good models to choose from, but testing the model can be very expensive, time-consuming, and even risky to the business. Recently, researchers and practitioners have started to fine-tune such large open-source models using techniques such as LoRA and QLoRA. Such methods allow one to adapt a large, open-source NN to a small dataset, and very cheaply. However, in fine-tuning, one could unwittingly overfit the model to the small dataset, degrading its performance for its intended use. Despite these and many other problems, theory remains well behind practice, and there is an increasingly pressing need to develop *practical predictive theory* to both improve the training of these very large NN models and to design new methods to make their use more reliable.

Before discussing these methods, however, let us explain *What is a Semi-Empirical Theory*

## 1.1 Statistical Mechanics (StatMech) vs. Statistical Learning Theory (SLT)

Historically, there have been two competing theoretical frameworks for understanding NNs: *Statistical Mechanics* (StatMech) [4, 5, 6, 7, 8, 9, 10]; and *Statistical Learning Theory* (SLT) [11].

- **Statistical Mechanics (StatMech).** This framework has been foundational to the early development of NN models, such as the Hopfield Associative Memory (HAM) [12], Boltzmann Machines [13], [14], etc. StatMech has also been used to build early theories of learning, such as the Student-Teacher model for the Perceptron Generalization Error [4, 5], the Gardner model [6], and many others. Notably, the HAM was based on an idea by Little, who observed that, in a simple model, long-term memories are stored in the eigenvectors of transfer matrix [15]. (This general idea, but in a broader sense, is central to our approach below.) Moreover, StatMech predicts that NNs exhibit phase behavior. This has recently been rediscovered as the Double Descent phenomenon [16, 17], but it was known in StatMech long before it’s recent rediscovery [18]. However, unlike other applied physics

theories (e.g., Semi-Empirical methods in quantum chemistry), **StatMech** only offers qualitative analogies, failing to provide testable quantitative predictions about large, modern NN models.[19]

- **Statistical Learning Theory (SLT)**. SLT and related approaches (VC theory, PAC bounds theory, etc.) have been developed within the context of traditional computational learning problems [11], and they are based on analyzing the convergence of frequencies to probabilities (over problem classes, etc.). It was recognized early on, however, that they could not be directly applied to NNs [20]. Moreover, SLT cannot even reproduce quantitative properties of learning curves [21, 22] (whereas **StatMech** is very successful at this [8]). SLT also failed to predict the “Double Descent” phenomenon [16]. More recently, it has been shown that in practical settings SLT can give vacuous [23] or even opposite results to those actually observed [24].

Technically, SLT focuses on obtaining bounds on a model’s worst-case behavior, while **StatMech** seeks a probabilistic understanding of typical behaviors across different states or configurations. Unfortunately, neither of these general theoretical frameworks has proven particularly useful to NN practitioners. **SETOL** combines insights from both. Rather than being purely phenomenological like the **HTSR** approach, **SETOL** is derived from first-principles, and in the form of a Semi-Empirical theory. As such, **SETOL** offers a practical, Semi-Empirical framework that bridges rigorous theoretical modeling and empirical observations for modern NNs.

## 1.2 Heavy-Tailed Self-Regularization (HTSR)

**HTSR** theory is an approach that combines ideas from **StatMech** with those of *Heavy-Tailed Random Matrix Theory* (RMT), providing eigenvalue-based quality metrics that correlate with model quality (i.e., out-of-sample performance). **HTSR** theory posits that well-trained models have extracted subtle correlations from the training data, and that these correlations manifest themselves in the *Shape* and *Scale* of the eigenvalues of the layer weight matrices  $\mathbf{W}$ . In particular, if one computes the empirical distribution of the eigenvalues,  $\lambda_i$ , of an individual  $N \times M$  weight matrix,  $\mathbf{W}$ , then this density,  $\rho^{emp}(\lambda)$ , which is an ESD, is Heavy-Tailed (HT) and can be well-fit to a *Power Law* (PL), i.e.,  $\rho(\lambda) \sim \lambda^{-\alpha}$ , with exponent  $\alpha$ . **HTSR** theory provides a *phenomenology* for qualitatively-distinct phases of learning [25]. It can, however, also be used to define *Layer-level Quality metrics* and *Model-level Quality metrics*: e.g., the **Alpha** ( $\alpha$ ) and **AlphaHat** ( $\hat{\alpha}$ ) PL metrics, described below.

Not needing any training data, **HTSR** theory has many practical uses. It can be directly applicable to large, open-source models where the training and test data may not be available. Model quality metrics can be used, e.g., to predict trends in the quality of SOTA models in computer vision (CV) [26] and natural language processing (NLP) [27, 28], both during and after training, and without needing access to the model test or training data. Layer quality metrics can be used to diagnose potential internal problems in a given model, or (say) to accelerate training by providing optimal layer-wise learning rates [29] or pruning ratios [30]. Most notably, the **HTSR** theory provides *Universal Layer Quality metrics* encapsulated in what appears to be a critical exponent,  $\alpha = 2$ , that is empirically associated with optimal or Ideal Learning. Moreover, as argued below, the value  $\alpha = 2$  appears to define a phase boundary between a generalization and overfitting, analogous to the phase boundaries seen in **StatMech** theories of NN learning.

These results both motivate the search for a first principles understanding of the **HTSR** theory, and suggest a path for developing a practical predictive theory of Deep Learning. For this, however, we need to go beyond the phenomenology provided by **HTSR** theory, to relate it to some sort of (at least semi-rigorous/semi-empirical) derivations based on the **StatMech** theory

of learning, and drawing upon previous success (in Quantum Chemistry) in developing a first principles Semi-Empirical theory.

### 1.3 What is a Semi-Empirical Theory?

Historically, one of the most well known *Semi-Empirical* methods comes from Nuclear Physics. The Semi-Empirical Mass Formula, dating back to 1935, is based on the heuristic Liquid Drop Model of the nucleus, and it was used to predict experimentally observed binding energies of nucleons. This model describes nuclear fission, and it was central to its development of the atomic bomb:

Prior to WWII, Nuclear Physics was a phenomenological science, which relied upon experimental data and descriptive models [31].

In the Post-war era, the epistemological nature of nuclear theory changed, as it saw the development of Semi-Empirical shell models of the nucleus. These models were formulated with rigor (in the physics sense) but also relied on heuristic assumptions and experimental data for accurate predictions. They captured the structure of atomic nuclei and could accurately describe various nuclear properties [32, 33, 34]. The shell models, analogous to the electronic shell structure of atoms, represented a shift toward a more rigorous understanding of nuclear phenomena.

About this time, RMT itself was also introduced by *Wigner* [35] to model the statistical patterns of the nuclear energy spectra of strongly interacting heavy nuclei. These patterns were universal, independent of the specific nucleus, suggesting that a probabilistic approach would be fruitful. In the following decades, RMT saw many advances, including the development of the Marchenko-Pastur model [36], and numerous other applications in physics [37]. By the 1990s, RMT was further expanded when *Zee* introduced the *Blue Function*, and reinterpreted the *R-transform* as a self-energy within the framework of many-body / quantum field theory (QFT) [38]. Also, so-called HCIZ integrals, integrals over random matrices, were being used both to model disordered electronic spectra [39], and, later, the behavior of spin glass models [40, 41].

Returning to the 1950s, and prior to the development of highly accurate, modern, computational *ab initio* theories of Quantum Chemistry, Theoretical chemists introduced the Semi-Empirical PPP method for conjugated polyenes [42]. The PPP model recasts the electronic structure problem as an *Effective Hamiltonian* for the  $\pi$ -electrons. The PPP model resembles the later developed tight-binding model of condensed matter physics [43]. For many years this and related Semi-Empirical methods worked remarkably well, even better than the existing *ab initio* theories [44, 45, 46, 47, 48]. Most importantly, these methods could be *fit* on a broad set of empirical molecular data, and then applied to molecules not in the original training set.

Around the same time, *Löwdin* first formalized the concept of the Effective Hamiltonian, which allowed the reduction of complex many-body problems to simplified *Effective Potentials* that still captured the essential physics. Then, in the late 1960s, Brandow developed an Effective Hamiltonian theory of nuclear structure, leveraging the *Linked Cluster Theorem* (LCT) (see [49]) and quantum mechanical many-body theory to describe the highly correlated effective interactions in a reduced model space.<sup>1</sup>

Like modern NNs, these Semi-Empirical methods of Quantum Chemistry worked well beyond their apparent range of validity, generalizing very well to out-of-distribution (OOD) data. This led to the search for a Semi-Empirical *Theory* to explain the remarkable performance of these

<sup>1</sup>Note also that the LCT shows that the log partition function (*i.e.*,  $\ln Z$ ) can be expressed as a sum of connected diagrams, which is very similar to our result below, which expresses the log partition function here as a sum of matrix cumulants from RMT.



phenomenological methods. Building on Brandow’s many-body formalism, Freed and collaborators [50, 51] developed an *ab initio* Effective Hamiltonian Theory of Semi-Empirical methods to explain the remarkable success of the Semi-Empirical methods. Specifically, the values of the PPP empirical parameters could be directly computed by way of effective interactions, including both renormalized self-energies and higher-order terms. Somewhat later, in the 1990s, Martin et. al. [52, 53, 54, 55] extended and applied this Effective Hamiltonian theory and demonstrated the Universality of the Semi-Empirical PPP parameters numerically. Indeed, it is this Universality that enabled the ‘for a time’ inexplicable OOD performance of these methods. Crucially, this decades-long line of work established a comprehensive analytic and numerical *Theory* of Semi-Empirical methods. That is, a framework that confirmed the empirically observed Universality provided theoretical justification for this, and enabled systematic improvements of the methods using numerical techniques.

Finally, it is important to mention the Effective Hamiltonian approach provided by the Wilson *Renormalization Group* (RG) [56, 57]. The RG approach provides a powerful framework for studying strongly correlated systems across different scales, enabling the construction of an Effective Hamiltonian by *integrating out* weakly-correlated degrees of freedom in a Scale-Invariant way. It is particularly suited for critical points and phase boundaries – such as the phase boundary between generalization and memorization in spin glass models of neural networks – and, importantly, predicts the existence of Universal Power Law (PL) exponents. For SETOL, we take what amounts to a single step of the *Exact Renormalization Group* (ERG), leading to a new empirical metric that defines the ‘Ideal’ NN layer.

**Relevance to Deep Learning** In this sense, Semi-Empirical theories of Nuclear Physics and Quantum Chemistry, (as well as the Renormalization Group approach), seem particularly appropriate for Deep Learning. DNN models are complex black boxes that defy statistical descriptions in that they are commonly pre-trained on a large set of data; and then applied to new data sets in new domains via transfer learning. Most recently, the inexplicable success of transfer-learning is seen in the GPT (Generative Pre-Trained Transformer) models [58], and motivated early work by Jumper et. al. on protein folding [59].

In contrast, these Semi-Empirical approaches differ from more recently developed theoretical approaches to deep learning, which are typically based on SLT, rather than **StatMech** [60]. In particular, there have recently appeared several theories of deep learning, formulated using ideas from RMT. However, regarding realistic models, it has been explicitly stated that “These networks are however too complex in general for developing a rigorous theoretical analysis on the spectral behavior” [61]. Even in recent work applying RMT to NNs, it has been noted “*that we make no claim about trained weights, only random weights*” [62]. The weight matrices of a trained NN, however, are clearly *not* simply random matrices—since they encode the specific correlations from the training data.

## 1.4 A Semi-Empirical Theory of Learning (SETOL)

We propose SETOL, a Semi-Empirical Theory for Deep Learning Neural Networks (NNs), as both a theoretical foundation for HTSR phenomenology and a novel framework for predicting the properties of complex NN models. This unified framework offers a deeper understanding of DNN generalization through a Semi-Empirical approach inspired by many-body physics, combined with a classic **StatMech** model for NN generalization. Specifically, SETOL combines theoretical and empirical insights to evaluate Model Quality, showing that the weightwatcher layer HTSR PL metrics (**Alpha** and **AlphaHat**) can be derived using a phenomenological Effective Hamiltonian approach. This approach expresses the HTSR Layer Quality in terms of the RMT matrix cumulants



of the layer weight matrix  $\mathbf{W}$ , and is governed by a Scale-Invariant transformation equivalent to a single step of an Exact Renormalization Group (ERG) transformation. Here, we derive this from first principles, requiring no previous knowledge of statistical physics.

The SETOL approach unifies the HTSR principles with a broader theoretical framework for layer analysis. The HTSR theory identifies Universality (e.g.,  $\alpha = 2$ ) as a hallmark of the best-trained DNN layers, and, here, our SETOL introduces the closely related *Exact Renormalization Group Condition*, a Scale-Invariant or Volume-Preserving transformation that reflects an underlying *Conservation Principle*. Together, these principles form the theoretical foundation for deriving HTSR Layer Quality metrics from first principles. By leveraging techniques from StatMech and modern RMT, SETOL offers a rigorous framework to connect empirical observations with theoretical predictions, advancing our understanding of generalization in neural networks.

- **Derivation of the HTSR Layer Quality metrics Alpha and AlphaHat.** The SETOL approach takes as input the Empirical Spectral Density (ESD) of the layers of trained NN, and derives an expression for the approximate *Average Generalization Accuracy* of a multi-layer NN. We call this approximation the *Model Quality*, denoted  $\bar{Q}^{NN}$ . This Model Quality is expressed as a product of individual Layer Quality terms,  $\bar{Q}_L^{NN}$ , which themselves can then be directly related to the HTSR Power Law (PL) empirical Alpha ( $\alpha$ ) and AlphaHat ( $\hat{\alpha} = \alpha \log_{10} \lambda_{max}$ ) metrics.

In particular, the Layer Quality-Squared,  $\bar{Q}^2 \approx [\bar{Q}_L^{NN}]^2$ , is expressed as the logarithm of an HCIZ integral, which is the Thermal Average of an Annealed Error Potential for a matrix-generalized form of the Linear Student-Teacher model of classical StatMech. This HCIZ integral evaluates into the sum of integrated R-transforms from RMT, or, equivalently, as a sum of integrated matrix cumulants. From this, the HTSR AlphaHat metric can be derived in the special case of Ideal Learning.<sup>2</sup>

- **Discovery of a Mathematical Condition for Ideal Learning.** By Ideal Learning, we mean that the specific NN layer has optimally converged, capturing as much of the information as possible in the training data without overfitting to any part of it. In defining this and deriving our results, we have discovered (and are proposing) a new condition for Ideal Learning, which is associated with the Universality of the HTSR theory:

- **HTSR Condition for Ideal Learning.** This HTSR theory states that a NN layer is Ideal when the ESD can be well fit to a Power Law (PL) distribution, with PL exponent  $\alpha = 2$ . Importantly, this appears to be a Universal property of all well-trained NNs, independent of the training data, model architecture, and training procedure.
- **SETOL ERG Condition for Ideal Learning.** The SETOL condition for Ideal Learning states that the dominant eigencomponents associated with the ESD of layer form a reduced-rank *Effective Correlation Space* (ECS) that satisfies a new kind of Conservation Principle, *Scale-Invariant Volume Preserving Transformation* where the largest eigenvalues  $\tilde{\lambda}_i$  of the ECS satisfy the condition  $\ln \prod \tilde{\lambda}_i = \sum \ln \tilde{\lambda}_i = 0$ . This is called the *ERG Condition*. The ERG Condition is equivalent to the taking a single step of the Wilson Exact Renormalization (ERG).

The HTSR Condition has been proposed and analyzed previously [25, 26, 28]; but the ERG Condition is new, based on our SETOL theory. When these two conditions align, we propose the NN layer is in the Ideal state.

<sup>2</sup>The SETOL approach to the HTSR theory resembles in spirit the derivation of the Semi-Empirical PPP models using the Effective Hamiltonian theory, where each phenomenological parameter is associated with a renormalized effective interaction, expressed as a sum of linked diagrams or clusters.[53, 55]

- 345 • **Experimental Validation.** We present detailed experimental results on a simple model,  
346 along with observations on large-scale pretrained NNs, to demonstrate that the HTSR con-  
347 ditions for ideal learning ( $\alpha = 2$ ) are experimentally aligned with the independent SETOL  
348 condition for ideal learning ( $\det(\tilde{\mathbf{X}}) = 1$ ). See Section. 6.3. Our primary objective here  
349 is not to demonstrate performance improvements on SOTA NNs—this has been previously  
350 established [29]. Instead, our aim is to **validate the theoretical assumptions** of SETOL,  
351 test the **predictions of the SETOL framework**, and examine the **new, independent**  
352 **learning conditions** we discovered—on a model that is sufficiently simple that we can  
353 evaluate and stress test the theory.
- 354 • **Observations on Overfit Layers ( $\alpha < 2$ ).** Being a Semi-Empirical theory, SETOL can also  
355 identify violations of it’s assumptions. For example, when empirical results show  $\alpha < 2$  for a  
356 single layer, the layer’s ESD falls into the HTSR Very Heavy-Tailed (VHT) Universality class.  
357 (See Section 6.6.) When this happens, the layer may be slightly overfit to the training data,  
358 resulting in **suboptimal performance** and potentially even exhibiting **hysteresis-like**  
359 **effects** (memory effects)—that we observe empirically. These effects indicate that overfit  
360 layers may retain memory-like behavior, affecting learning dynamics and generalization.

## 2 Heavy-Tailed Self-Regularization (HTSR)

In this section, we provide an overview of the HTSR phenomenology.<sup>3</sup> HTSR has been presented in detail previously [63, 64, 25]. Here, we provide a self-contained summary, with an emphasis on certain technical issues that will be important for our SETOL. We highlight its practical application for interpreting observed behaviors in trained weight matrices, and we distinguish the HTSR phenomenology from the analytical methods used in the SETOL approach. In Section 2.1, we summarize the basic HTSR setup and results; in Section 2.2, we summarize Gaussian (for RMT) and Heavy-Tailed (for HTRMT) Universality; and in Section 2.3, we describe *Shape* metrics and *Scale* metrics that arise from HTSR. (Here, we focus on basic methods for identifying HT correlations in the ESDs of pre-trained weight matrices; in Sections 6.1, 6.5 and 6.6, we show detailed experiments using theoretical constructs from the HTSR phenomenology.)

### 2.1 The HTSR Setup

We can write the Energy Landscape function (or NN output function) for a NN with  $L$  layers as

$$E_{NN}^{out} := h_L(\mathbf{W}_L \times h_{L-1}(\mathbf{W}_{L-1} \times (\dots) + \mathbf{b}_{L-1}) + \mathbf{b}_L) \quad (1)$$

with activation functions  $h_l(\cdot)$ , and with weight matrices and biases  $\mathbf{W}_l$  and  $\mathbf{b}_l$ .<sup>4</sup> For simplicity of exposition here (HTSR can be applied much more broadly), we ignore the structural details of the layers (dense or not, convolutions or not, residual/skip connections, etc.). We also ignore the biases  $\mathbf{b}_l$  (because they can be subsumed into the weight matrices), and we treat each layer as though it contains a single weight matrix  $\mathbf{W}_L$ . We imagine training (or fine-tuning) this model on labeled data  $\{\mathbf{x}_\mu, y_\mu\} \in \mathcal{D}$ , where  $\mathbf{x}_\mu$  is the  $\mu$ -th input vector and  $y_\mu$  is its corresponding label (e.g., for binary classification,  $y_\mu \in \{-1, 1\}$ ). We expect to use backprop via some variant of stochastic gradient descent (SGD) to minimize some loss functional,  $\mathcal{L}$  (such as  $\ell_2$ , cross-entropy, etc.):

$$\operatorname{argmin}_{\mathbf{W}_l, \mathbf{b}_l} \sum_{\mu} \mathcal{L}[E_{NN}^{out}(\mathbf{x}_\mu), y_\mu] + \Omega, \quad (2)$$

where  $\Omega$  denotes some explicit regularizer (such as an  $\ell_1$  or  $\ell_2$  constraint on layer weight matrices) or some implicit regularization procedure (such as clipping the weight matrices or applying dropout).

Given a real-valued  $N \times M$  layer weight matrix  $\mathbf{W}$  (dropping the subscript), let  $\mathbf{X}$  be the  $M \times M$  layer *Correlation Matrix*:

$$\mathbf{X} := \frac{1}{N} \mathbf{W}^\top \mathbf{W}. \quad (3)$$

The Empirical Spectral Density (ESD) of  $\mathbf{W}$ , denoted  $\rho^{emp}(\lambda)$ , is formed from the  $M$  eigenvalues  $\lambda_j$  of  $\mathbf{X}$ :

$$\rho_{emp}(\lambda) := \sum_{j=1}^M \delta(\lambda - \lambda_j). \quad (4)$$

Given a model, we can compute the ESDs of all of its layers, as well as other metrics below, with the open-source **WeightWatcher** tool [67].<sup>5</sup>

<sup>3</sup>We may also refer to the HTSR phenomenology as the HTSR Theory; we use the term phenomenology to emphasize its empirical nature, and to distinguish it from the analytical methods used in the SETOL approach.

<sup>4</sup>The Energy Landscape function  $E_{NN}^{out}$  acts on a data instance and generates a list of energies, or un-normalized probabilities; [25]. This notation was chosen to make an analogy with Random Energy Models (REM) from spin-glass and protein folding theories [65, 66].

<sup>5</sup>For practical purposes, the **WeightWatcher** tool computes  $\rho^{emp}(\lambda)$  by forming the Singular Value Decomposition (SVD) of the layer weight matrices  $\mathbf{W}$ , computing the eigenvalues  $\lambda = \sigma^2$  from the singular values  $\sigma$ , and (when useful) smoothing them with a Kernel Density Estimator (KDE). For some calculations, such as the ERG condition, we must also select the appropriate normalization of  $\mathbf{W}$ .

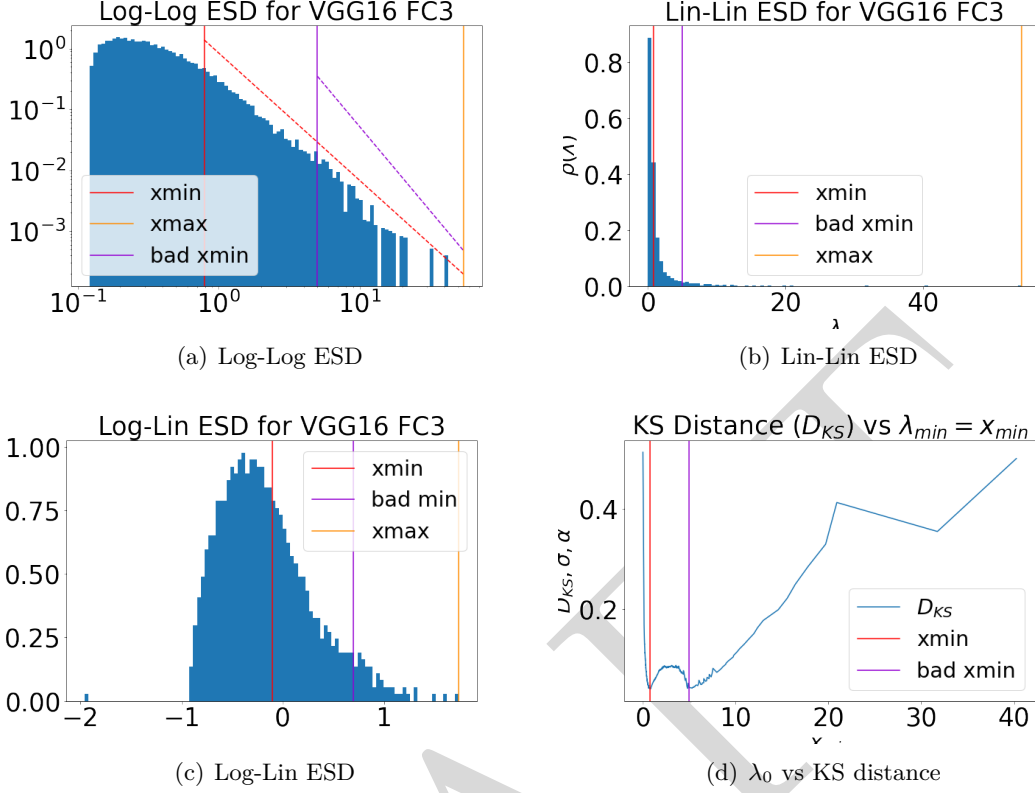


Figure 1: **Fitting ESDs within HTSR.** Depiction of the ESD and results of PL fits for a typical well-trained layer of a modern NN (FC3 of VGG19), including both the actual and good PL fit (red) and a hypothetical bad PL fit (purple). The same ESD is plotted on a Log-Log (a), Lin-Lin (b) and Log-Lin (c) scales. (d) depicts how the start of the PL tail,  $\lambda_0$ , varies with the quality of the PL fit (the  $D_{KS}$  distance). All plots are generated using the open-source **WeightWatcher** tool. See the main text for details.

Based on empirical results based on thousands of pretrained models and tens of thousands of layers [25, 26, 24, 28], it is generally observed that the best performing NNs have ESDs that are HT, and the *tails* of these ESDs,  $\rho_{tail}(\lambda)$ , can be well fit to a PL, beyond some cutoff  $\lambda \geq \lambda_0$ .<sup>6</sup> For a PL fit,

$$\rho_{tail}(\lambda) := \rho^{emp}(\lambda \geq \lambda_0) \sim \lambda^{-\alpha}, \quad (5)$$

where  $\lambda_0$  is where the tail of the ESD starts (i.e., it is not the minimum eigenvalue, but the minimum eigenvalue in the tail of the ESD). See Figure 1. As such, the tail of the ESD “starts” at some value  $\lambda_0$ , called *xmin* here, and it continues until the maximum eigenvalue  $\lambda_{max}$ , called *xmax* here (labeled *xmax* in the figure, shown by the orange line). We estimate *xmin* and  $\alpha$  jointly, using the method of [68], as implemented in the **powerlaw** python package [69], which is also integrated into the open-source **WeightWatcher** tool [26, 67].<sup>7</sup>

<sup>6</sup>Doing a large meta-analysis like this is tricky; but see [25, 26, 24, 28]. The **WeightWatcher** tool provides a systematic, reproducible way to compute a PL fit (using an MLE method of Clauset et al. [68]), as well other model metrics, including the **SpectralNorm**, **Rand-Distance**, and **AlphaHat** metrics [26]. Also, the ESD  $\rho(\lambda)_{tail}$  is sometimes better fit by a Truncated Power Law (TPL), due to finite-size effects. (Again, this is important in practice, but we ignore this complexity in this initial discussion of SETOL.)

<sup>7</sup>The authors of [70] failed to find evidence of a PL-like distribution in NN weight matrices, which is likely to be the case when  $\alpha$  and *xmin* are not estimated *jointly*, as can be seen in Figure 1(d).

HT/RMT Universality class	$\mu$ range	$\alpha$ range	Best Fit
RandomLike	NA	NA	MP
Bulk+Spikes	NA	NA	MP+Spikes
Weakly Heavy Tailed	$\mu > 4$	$\alpha > 6$	PL
Heavy (Fat) Tailed	$\mu \in (2, 4)$	$\alpha \in (2, 6)$	PL
Very Heavy Tailed	$\mu \in (0, 2)$	$\alpha \in (1, 2)$	(T)PL
Rank Collapse	NA	NA	NA

Table 1: HTSR Heavy-Tailed Universality classes of RMT. See Table 1 of [25] for more details.

**Fitting ESDs.** Choosing the start of the tail,  $\lambda_0$ , is important for HTSR (and it will be very important for SETOL, as we will describe below). See Figure 1 for a depiction of how this was done within HTSR theory. Figures 1(a)-1(c) show the results of both a “good fit” and a “bad fit” on the same ESD, while Figure 1(d) indicates the quality of fit. For the good fit, the start of the tail is the optimal value  $\lambda_0 = x_{min}$  (in red); and for the bad fit, it is a suboptimal *bad xmin* (purple). Figure 1(d) depicts how the best fit is determined; it plots  $x_{min} = \lambda_0$  versus the  $D_{KS}$  value, which is the Kolmogorov-Smirnov (KS) distance between the PL fit and the empirical data [68]. Notice that there are two nearly degenerate minima on Figure 1(d), corresponding to the good fit and the bad fit. It is not uncommon to face such practical challenges, as real-world ESDs are often slightly deformed from a perfect PL density, e.g., they may have two or more near-degenerate solutions on the KS plots (d). (They may also have anomalously large eigenvalues; this is discussed in more detail in Section 3.3.)

When one finds a good PL fit for the ESD of a layer  $\mathbf{W}$ , it provides information about the *Shape* and *Scale* of the ESD of that layer. In particular: the **SpectralNorm**,  $\lambda_{max}$ , being a matrix norm, is a measure of the size *Scale* of the ESD [24]; the fitted PL exponent **Alpha**,  $\alpha$ , being the slope of the tail of the ESD on a Log-Log plot, describes the *Shape* of the ESD; and the **WeightWatcher AlphaHat** metric combines *Shape* and *Scale* information. Also, as opposed to other applications of PL fits [68, 71], in our analysis, the start of the tail,  $\lambda_0 = \lambda_{min}^{PL}$ , plays a particularly important role because it identifies the subspace of the strongest generalizing eigencomponents (i.e.,  $\tilde{\mathbf{X}}$ , below) in each layer.

## 2.2 Gaussian and Heavy-Tailed Universality

The HTSR phenomenology uses RMT to classify of the ESD of a layer  $\mathbf{W}$  into one of 5+1 Phases of Training, each roughly corresponding to a (Gaussian or HT) Universality class (of RMT or HTRMT). This is summarized in Table 1. A Universality class is a set of matrices having a common limiting spectral distribution, regardless of the other properties of their entries. Of those, the most familiar is the Gaussian class, characterized by the Marchenko Pastur (MP) results from traditional RMT [72, 73]. The Gaussian Universality class, however, is particularly poorly suited for analyzing realistic NNs—precisely because the ESDs of SOTA NNs are well-fit by HT distributions. This should not be surprising: weight matrices of realistic NNs do *not* have independent (i.i.d.) entries—their entries are strongly-correlated precisely because they provide a view into the correlated training data.

To model strongly-correlated NN layer matrices, the HTSR phenomenology characterizes NN layer weight matrices in terms of their ESDs (when a good PL fit can be found) by postulating that the (tail of the) eigenvalue spectrum  $\rho(\lambda)$  determines how each layer contributes to the overall generalization. To do this, the HTSR approach models the strong-correlated layer weight matrices *as if* they are actually i.i.d. HT random (i.e., entry-wise uncorrelated) matrices. By



Figure 2: MP distributions for different aspect ratios  $Q$  and variance scales  $\sigma^2$ , and an example of the finite-sized TW fluctuation  $\Delta_{TW}$ .

doing this, one can associate each  $\rho(\lambda)$  with the corresponding HT Universality class, according to the PL exponent  $\alpha$  fitted from the ESD. As we will see in Section 3.3, it can be critical to distinguish when the ESD is HT *Correlation-wise* vs HT *Element-wise*.

To understand Table 1 better, we first review basic results.

### 2.2.1 Random Matrix Theory (RMT): Marchenko-Pastur (MP) Theory and Tracy-Widom (TW) Fluctuations

The Marchenko-Pastur (MP) distribution predicts the (limiting) *Shape* of an ESD,  $\rho_{MP}(\lambda)$ , when the layer weight matrix has elements that are i.i.d. random from the Gaussian Universality class. In particular, the ESD will be MP when the matrix elements are drawn from a Normal distribution  $W_{i,j} \in N(0, \sigma^2)$ , e.g., as is typical at initialization, before NN training begins. Figure 2 (from Figure 4 of [25]) displays the MP distribution for different aspect ratios  $Q = \frac{N}{M}$  and variances  $\sigma^2$ . Notice that the *Shape* is characterized by a well-defined, compact envelope with sharp edges.

The MP distribution also predicts the *Scale* of an ESD, again when the layer weight matrix has elements that are i.i.d. random from the Gaussian Universality class. In particular, an MP distribution,  $\rho_{MP}(\lambda)$ , has very crisp, well-defined lower and upper bounds  $\lambda^-, \lambda^+$  [25], and (importantly) the upper bound  $\lambda^+$  exhibits finite-size Tracy-Widom (TW) fluctuations,  $\Delta_{TW}(\lambda)$ , which are on the order of  $\mathcal{O}(M^{-2/3})$ . Thus, any layer eigenvalue with *Scale* greater than this, i.e.,  $\lambda > [\lambda^+ + \Delta_{TW}(\lambda)]$ , is an “outlier” or a “spike.”

According to the HTSR phenomenology, these spikes carry significant generalizing information. (This is well-known for Bulk-Plus-Spike models [25], but the HTSR phenomenology generalizes this concept.) Relatedly, for layer matrices  $\mathbf{W}$  with aspect ratio  $Q > 1$  (i.e., rectangular matrices, where  $N > M$ ), MP RMT predicts there should be no zero eigenvalues, i.e.,  $\lambda_i > 0$ , for all  $i$ . Generally speaking, for well trained NNs, for layers with  $Q > 1$ , all eigenvalues are strictly larger than zero, i.e., well-trained layer weight matrices, with  $Q > 1$ , should have full rank and exhibit no “rank collapse.” HTSR places random Gaussian and “Bulk-Plus-Spike” matrices into the first two rows of Table 1. The essential feature of Gaussian random matrices is that their entries have no correlations. When some correlations are injected, a few large spike eigenvalues form, without otherwise disturbing the shape of the ESD. To really understand how individual NN layers converge, we need to understand when and why their ESDs become HT.



### 2.2.2 Heavy-Tailed Random Matrix Theory (HTRMT) and Power Law (PL) fits

For very well-trained NN layers, ESDs are *not* MP at all. Frequently, if not always, their ESDs are HT—and they are HT *because* they are strongly-correlated matrices. Importantly, they are *not* HT element-wise. Instead, their entries have a scale, and they have ESDs that are HT due to correlations learned during training. Existing theoretical approaches, including SLT and even StatMech, cannot readily model such strongly-correlated systems.<sup>8</sup>

Such strongly-correlated systems, however, do frequently arise in other, related scientific domains, including in the StatMech of self-organizing systems [76, 77], in electronic structure theory [53, 55, 54], and in quantitative finance [78, 79, 73]. In these (and other) domains, correlated systems frequently exhibit characteristic PL signatures; and it is common practice to *model* correlated systems as random (uncorrelated) systems by using HT statistics (e.g., Levy distributions or PL random matrices), fully understanding that such systems are by no means actually i.i.d. random. The HTSR phenomenology builds upon this longstanding practice by delimiting families of HT NN weight matrices based on the corresponding Universality classes of Pareto matrices.

We explain briefly how to interpret Table 1 with respect to HTRMT. The 5+1 Phases of Training can be identified by fitting ESDs to MP or PL distributions, whichever gives the best fit, as shown in the last column. In case the PL distribution is a better fit, HTSR phenomenology treats the layer weight matrix as equivalent to an i.i.d. random matrix  $\mathbf{W}(\mu)$ , whose elements have been drawn from a Pareto distribution with exponent  $\mu$ .

**Heavy-Tailed Universality Classes of Random Pareto Matrices** For such an element-wise HT matrix, the theoretical *limiting* ESD of a Pareto matrix is also PL, which allows us to related the fitted PL  $\alpha$  with exponent  $\alpha = a\mu + b$ , to the Pareto exponent  $\mu$ . Ideally, for an infinite width matrix,  $a = \frac{1}{2}$  and  $b = 1$ , but due to finite-size effects, however, we have found we must take  $a \geq \frac{1}{2}$  and  $b \geq 1$ , giving

$$W_{i,j}(\mu) \sim \frac{C}{x^{\mu+1}}, \quad \rho(\lambda) \sim \lambda^{-(a\mu+b)}. \quad (6)$$

According to the above relation, we can use either the fitted PL exponent  $\alpha$ , or the Pareto exponent  $\mu$ , to index the HT Universality classes, Note, however, that the finite-size effects strongly depend on the aspect ratio  $Q = N/M$ , at least when applied to i.i.d random Pareto matrices, and the (Clauset MLE) PL fit may overestimate the  $\alpha$  of the ESD. Table 1 delimits the HT matrices into sub-categories (as shown in the bottom four rows) based on the behaviors of  $\alpha$  as a function of  $\mu$ .

Figure 3 illustrates how the fitted PL exponent  $\alpha$  corresponds to the actual Pareto exponent  $\mu$  for different aspect ratios  $Q = M/M$ . Figure 3(a) displays the ESDs of three different i.i.d.  $1000 \times 1000$  HT random matrices, with  $\mu = 1, 3, 5$ , on a Log-Log scale. Notice that smaller  $\mu$ , and therefore smaller  $\alpha$ , corresponds to heavier (i.e., larger) tails. Figure 3(b) shows how the empirically fit PL exponent  $\alpha$  can vary with the theoretical  $\mu$  for an associated  $\mathbf{W}(\mu)$ . For  $\mu < 2$  and  $Q = 1$ , the fitted  $\alpha$  follows the linear relation  $\alpha = \frac{1}{2}\mu + 1$ , albeit with some error. In contrast, for the more relevant  $\mu \in (2, 4)$  regime, the relation now depends far more strongly on the aspect ratio  $Q$ , and  $\alpha \in [2, 6]$ . For  $\mu > 4$ , the fitted  $\alpha$  saturates for each specific value of  $Q$ .

We emphasize that we only model the ESDs of the NN layer weight matrices using the same Universality class to that associated with the ESD of a random, i.i.d, HT Pareto matrix. In fact, the elements  $W_{i,j}$  do not at all appear as if they have been drawn from an HT Pareto distribution,

<sup>8</sup>For example, such theoretical approaches typically deal better with *Scale* information (such as  $\lambda_{max}$ ) than with *Shape* information (such as  $\alpha$ ), e.g., by characterizing an “eigen-gap” separating large eigenvalues from “noise” [74] according to a noise plus low-rank perturbation model [75].

and, in contrast, are almost always well fit to a Laplacian distribution. Also, despite these strong finite-size effects, empirically one finds that the ESDs arising large, well trained, modern NNs can frequently be well fit to a PL (or TPL), and that the fitted  $\alpha \in [2, 6]$  for 80 – 90% of NN layers. Notably, we rarely find  $\alpha < 2$  in the best performing, open source, pretrained DNNs.

As there is *no* ground truth whatsoever as to the limiting spectral density of a strongly-correlated NN weight matrix (especially without HT elements) the HTSR phenomenology uses Pareto matrices as a guide. However, as we will see in Section 3.3, this analogy should be treated with caution because there are cases where it breaks down.

No matter why a matrix ESD is HT, it can be difficult to reliably estimate the  $\alpha$  parameter when the true  $\alpha$  is large. For Pareto matrices of the size investigated here, an observed  $\alpha$  above 6 is uninformative — the tail will decay very rapidly indeed, leaving very little of it to study. In this sense, the HT Universality classes are *larger* than the set of only strongly-correlated matrices or Pareto random matrices.

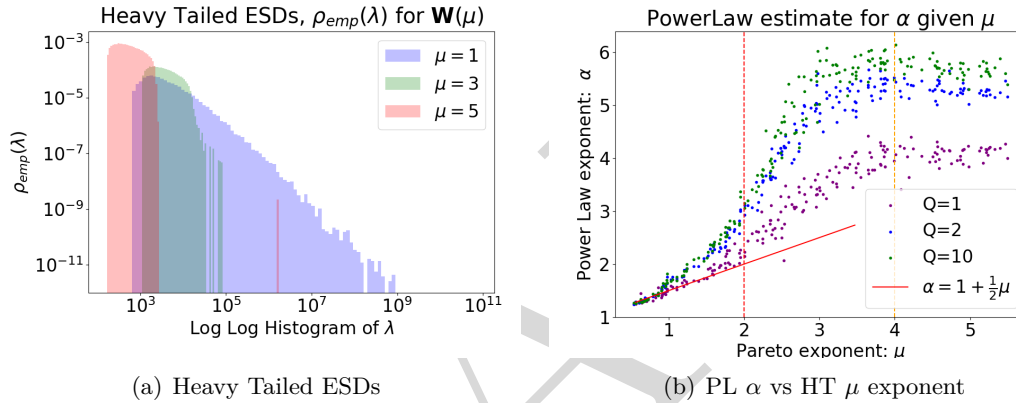


Figure 3: Comparison of ESDs and Power Law (PL) exponents  $\alpha$  from Heavy-Tailed (Pareto) weight matrices  $\mathbf{W}(\mu)$ . Subfigure (a) depicts 3 typical ESDs with Pareto exponent  $\mu = 1, 3, 5$ , each decreasing in *Shape* and *Scale*. Subfigure (b) shows how the exponent  $\alpha$  of the PL fit varies with  $\mu$ , with significant finite-size effects emerging for  $\mu > 2$  and  $\alpha > 2$ .

There is a particularly important boundary between Universality classes where  $\alpha = 2$ . Recall that one of the properties of power law distributions  $\rho(\lambda) \sim \lambda^{-\alpha}$  is that if  $\alpha < 2$ , then the variance of  $\rho(\lambda)$  is infinite. In such cases, the variance cannot be estimated empirically, making  $\rho(\lambda)$  in some sense *atypical*. This implies that the NN will have substantially greater difficulty in applying any further load to such a weight matrix. Thus, the value of  $\alpha = 2$  is a *critical value*. (See Figure 27 in Section 6.6 for an empirical study of this effect in a small MLP.)

Smaller PL exponent  $\alpha$  values correspond to heavier tails,  $\rho_{tail}(\lambda)$ ; and the HTSR phenomenology observes that smaller PL exponents  $\alpha$  (at least for  $\alpha \in (2, 6)$ ) tend to correspond to better models. This is the key idea of the HTSR: the generalizing components of a layer matrix  $\mathbf{W}$  concentrate in larger singular vectors associated with the tail, and so that better models have more slowly-decaying (i.e., larger) ESD tails. This differs significantly than simply taking a general low-rank approximation to  $\mathbf{W}$ , where the rank is chosen without insight from the HTSR phenomenology. The SETOL theory formalizes this observation as a key assumption. We will revisit these model selection questions in Section 3.1 below.

### 2.3 Data-Free *Shape* and *Scale* Quality Metrics

The HTSR phenomenology provides quality metrics for both individual layers and (by averaging layers) for an entire NN model.

**Layer-wise Quality Metrics.** Using the HTSR phenomenology, we can define several other *Shape* and/or *Scale* based layer (quality) metrics. These are available in the **WeightWatcher** tool, and they work very well in practice.

- **Alpha** ( $\alpha$ ):  $\rho_{tail}(\lambda) \sim \lambda^{-\alpha}$ . A *Shape*-based quality metric.
- **LogSpectralNorm**:  $\log_{10} \lambda_{max}$ . A *Scale*-based quality metric.
- **AlphaHat** ( $\hat{\alpha}$ ):  $\alpha \log_{10} \lambda_{max}$ . A *Scale*-adjusted *Shape*-based quality metric.
- **Rand-Distance**:  $JSD[\rho^{emp} | (\rho_{rand}^{emp})]$ . A *Shape*-based, non-parametric quality metric, suitable for highly-accurate, epoch-by-epoch analysis.<sup>9</sup>
- **PL KS**:  $D_{KS}$ . The KS-distance, or quality-of-fit, of the PL fits. For transformers, foundation models, and large, complex, modern NNs, this is frequently an even better model quality metric than the  $\alpha$  of the PL fit itself.
- **MP SoftRank**:  $\mathcal{R}_{MP}$ . The MP-SoftRank, defined in [25], can be used to identify problems such as when there is significant label or data noise that causes spuriously small  $\alpha$ , and also when it is difficult to fit a PL law.<sup>10</sup>

Each of these quality metrics provide a simple characterization of the *Shape* and/or *Scale* of the tail of the ESD of a given layer  $\mathbf{W}$ . These metrics are related to each other, and they have various trade-offs in practice [26, 24, 28]. Of particular interest here in our development of SETOL are the PL-based **WeightWatcher Alpha** and **AlphaHat** metrics.

**From Layer-wise Quality Metrics to Layer-Averaged Model Quality Metrics.** One can use the HTSR phenomenology to go beyond individual Layer Quality metrics, to construct model quality metrics by averaging Layer Quality metrics (over all layers that are not very small). Existing HTSR model quality metrics implicitly require that all layers are statistically independent, so that the average model quality is just the average of the contributions from each weight matrix  $\mathbf{W}$ .<sup>11</sup> Given a Layer Quality metric,  $\bar{\mathcal{Q}}_L^{NN}(\mathbf{W})$ , one can define the *Model Quality*  $\bar{\mathcal{Q}}^{NN}$  metric for an entire model as

$$\bar{\mathcal{Q}}^{NN} := \prod_L \bar{\mathcal{Q}}_L^{NN}(\mathbf{W}), \quad (7)$$

a product of each independent Layer Quality  $\bar{\mathcal{Q}}_L^{NN}$ , and then consider the layer average as the *log Layer Quality*,

$$\log \bar{\mathcal{Q}}^{NN} = \frac{1}{N_L} \sum_L \log \bar{\mathcal{Q}}_L^{NN} = \langle \log \bar{\mathcal{Q}}_L^{NN} \rangle_{\bar{L}} \quad (8)$$

<sup>9</sup>JSD is the Jensen-Shannon Divergence between the original ESD and the ESD of the layer weight matrix, randomized element-wise.

<sup>10</sup>The **WeightWatcher** tool also implements the WW-SoftRank, which is like the MP-SoftRank, but replaces  $\lambda_{bulk}^+$  with  $\lambda_{rand}^{max}$ ; these are mostly equivalent for large matrices, but they can be different for very small matrices.

<sup>11</sup>This independence assumption, clearly a mathematical convenience, gets us closer to a workable theory. One could go beyond a “single layer theory” by adding in intra-layer correlations empirically. The **WeightWatcher** tool does support this, but doing so is outside the scope of this work.

564 where  $\langle \dots \rangle_{\bar{L}}$  denotes the layer average.

565 In particular, prior work has used the following metrics:

- 566 • The layer-averaged model quality metric **Alpha**,  $\log \bar{Q}^{NN} = \langle \alpha \rangle_{\bar{L}}$ , describes the *Shape* of the  
 567 ESDs. One can use the averaged **Alpha** when studying a single model, and only varying  
 568 the regularization hyperparameters, although **Alpha** also works very well as a model quality  
 569 metric when comparing different transformer models [80].
- 570 • The layer-averaged model quality metric **LogSpectralNorm**,  $\log \bar{Q}^{NN} = \langle \log \lambda_{max} \rangle_{\bar{L}}$ , de-  
 571 scribes the *Scale* of the ESDs. The averaged **LogSpectralNorm** does work as a model  
 572 quality metric, but not as well as **Alpha** (or **AlphaHat**). Notably, **SLT** predicts that smaller,  
 573 not larger, **LogSpectralNorm** should be correlated with model quality; the opposite is ob-  
 574 served in practice! This is because a smaller layer  $\alpha$  generally, but not always, corresponds  
 575 to a larger  $\lambda_{max}$ .<sup>12</sup>
- 576 • The layer-averaged model quality metric **AlphaHat**,  $\log \bar{Q}^{NN} = \langle \alpha \log \lambda_{max} \rangle_{\bar{L}} = \langle \hat{\alpha} \rangle_{\bar{L}}$ , incor-  
 577 porates both *Shape* and *Scale* information. This can compensate for anomalies that can  
 578 arise when (say) comparing models of different sizes or model qualities [24] or when other  
 579 issues cause unusually large  $\lambda_{max}$ . See Section 3.3.1).

580 The layer-averaged **AlphaHat** model quality metric has been applied in a large meta-analysis of  
 581 hundreds of SOTA pre-trained publicly-available NN models in CV and NLP [26, 27, 28, 81].  
 582 Generally speaking, HTSR shape-based metrics, when used appropriately, outperform all other  
 583 metrics studied (including those from **SLT**, and with access to the training/testing data,) for  
 584 predicting the quality of SOTA pre-trained publicly available NN models. The HTSR theory  
 585 predicts that the best-performing NN models have layers with **Alpha**  $\in [2, 6]$ , and with  $\alpha = 2$   
 586 indicating optimal performance. Moreover, prior empirical results show that the **Alpha** and  
 587 **AlphaHat** metrics can predict trends in the Quality (i.e., the Generalization Accuracy), of SOTA  
 588 NN models—even without access to any training or testing data [26].

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<sup>12</sup>The **LogSpectralNorm** can exhibit a Simpson’s paradox when segmenting models by quality) [24]. Nevertheless, this metric may be useful when a PL fit can not be obtained, say, when  $N \gg M$  and  $M$  is very small, as with LSTMs, U-Net architectures, etc.

### 3 A Semi-Empirical Theory of (Deep) Learning (SETOL)

Based on prior empirical results, and the success of the **Alpha** and **AlphaHat** metrics that are based on the HTSR phenomenology, this leads to the deeper question:

*Why do the **Alpha** and **AlphaHat** metrics work so well as NN model quality metrics for SOTA NN models?*

That is, why do NN models with heavier-tailed layer Empirical Spectral Distributions (ESDs) tend to generalize better when compared to related models, and how can single-layer metrics predict model quality so well? Relatedly, can we derive these metrics from first principles? (If so, then under what conditions do they hold, and under what conditions do they fail?) To answer these questions, we will derive a general expression for the Layer Quality,  $\bar{Q}$ , of an NN. Although many modern NNs have many layers, we adopt a single-layer viewpoint (like a matrix-generalized Student-Teacher) because in Statistical Mechanics of Generalization (SMOG) theory [8, 82] the multi-layer generalization can be factorized or approximated. For this, we will obtain by simple averaging our model quality metrics, under effectively a single layer approximation, that correspond to **Alpha** and **AlphaHat**.

In deriving these quantities, we will introduce to NN theory a new Semi-Empirical approach that combines techniques from **StatMech** and **RMT** in a novel way. must depend on the spectral density The Layer Quality  $\bar{Q}$  will estimate the contribution that an individual NN layer makes to the overall quality of a trained NN model. In deriving  $\bar{Q}$ , we have discovered a new Layer Quality metric, called the **ERG** condition, which indicates that the generalizing components of the layer must concentrate into a low-rank subspace which we term the *Effective Correlation Space*, or **ECS**. That is, the better this condition is met, the more the generalizing components concentrate in this **ECS**, and this tendency provides a new layer quality metric, derived in a totally independent way from **Alpha** and **AlphaHat**. We will provide strong empirical justification that both metrics are acceptable Quality metrics by showing that they converge as model quality increases.

Importantly, we have conducted detailed experiments to show that the empirical estimates of the **SETOL** **ERG** condition align remarkably well with predictions from the HTSR theory under Ideal conditions (see Sections 6.1) and, then, that the key assumptions of our **SETOL** theory are valid (see Sections 6.2 and 6.3). In Section 6.4, we demonstrate how to apply theory directly using explicit calculations of the **RMT** layer cumulants. We next examine how the HTSR predictions (i.e., the HT PL exponent  $\alpha$ ) behave under non-Ideal conditions (see Sections 6.5 and 6.6). In the following, we will outline key conceptual aspects of **SETOL**. In Section 3.1, we give an overview of **SETOL**; In Section 3.2, we describe the conditions of Ideal learning under **SETOL** and how they differ from those of HTSR; and In Section 3.3 we describe conditions that deviate from this.

#### 3.1 SETOL Overview

Our **SETOL** formulates a parametric expression for the Layer Quality  $\bar{Q}$  using a matrix-generalization of the classic Student-Teacher (ST) model from the **SMOG** theory of the 1990s [8, 82], but with a Semi-Empirical twist in that the Teacher is now an actual, trained NN that is input to theory. Recent advances in the evaluation of so-called HCIZ random matrix integrals [73, 83, 84], such that the final expression for  $\bar{Q}$  to be written in terms of empirically measured statistical properties of the layer ESD. We summarize our basic approach here; see Section 5 for a detailed derivation, and see Section 6 for a detailed empirical analysis. For reference here and later, Figure 4 displays a flowchart of the conceptual development of **SETOL**.

As is done in the Student-Teacher (ST) model [8], we first formulate the Generalization Error ( $\bar{\mathcal{E}}_{gen}^{ST}$ ) of the linear Perceptron (in the *Annealed Approximation*, and in the *High-Temperature*

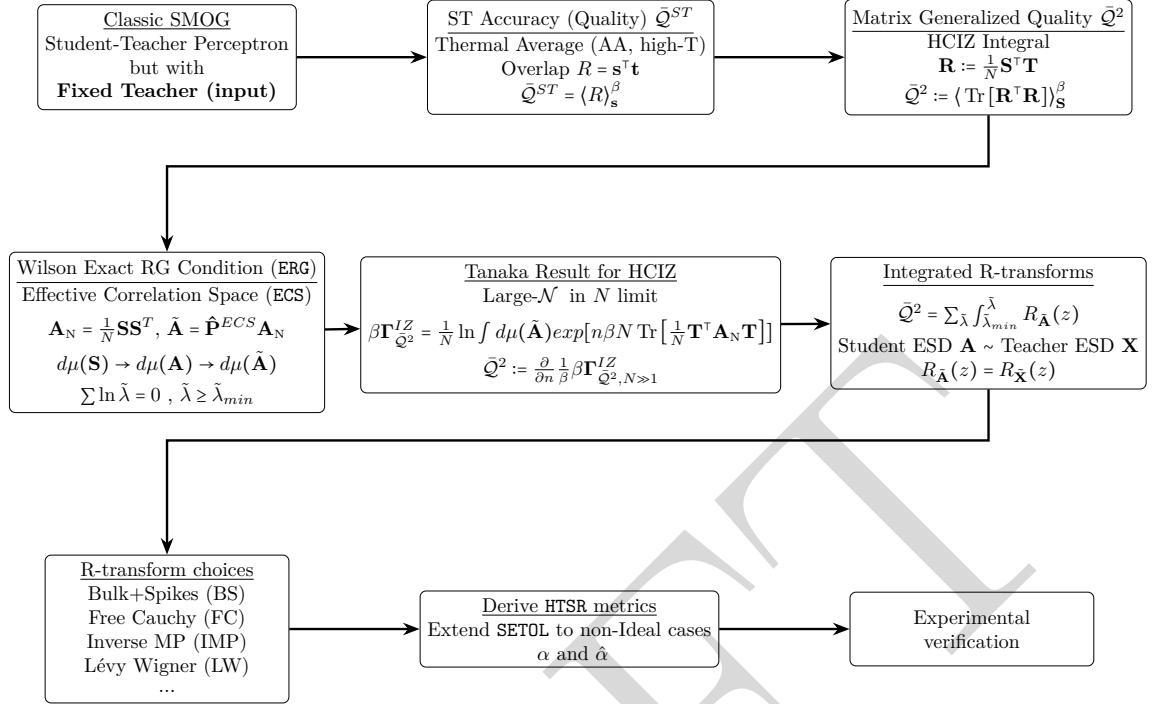


Figure 4: Flowchart of the theoretical concepts used to construct SETOL.

limit; see Section 4), and we then generalize this to the case of a NN ( $\bar{\mathcal{E}}_{gen}^{ST} \rightarrow \bar{\mathcal{E}}_{gen}^{NN}$ ), so that we can analyze the Quality of each layer. For the Perceptron, the Generalization Error is an Energy, given as  $\bar{\mathcal{E}}_{gen}^{ST} := \langle 1 - R \rangle_s^\beta$ , where  $R$  is the ST vector overlap, and  $\langle \dots \rangle_s^\beta$  is a *Thermal Average* (defined in Section 4.2), a Boltzmann-weighted average. In this case, the model Quality,  $\bar{Q}^{ST}$  is exactly the AA, high-T Average Generalization Accuracy  $\bar{Q}^{ST} := 1 - \bar{\mathcal{E}}_{gen}^{ST} = \langle R \rangle_s^\beta$ . For an MLP or general NN, each layer's Energy is (negatively) associated with a Layer Quality  $\bar{Q}$ , which we identify as the average contribution an individual layer contributes to the overall generalized accuracy, (i.e  $1 - \bar{\mathcal{E}}_{gen}^{NN}$ ) for a multilayer perceptron (MLP).

**Importantly, we deviate from the traditional approach in that we take the Teacher as a fixed, empirical input to the theory.** The Teacher contribution is then formulated in terms of the actual the layer eigenvalues, or Empirical Spectral Density (ESD). In this way, the theory becomes Semi-Empirical.

For technical reasons (below), we will seek the *Layer Quality (Squared)*  $\bar{Q}^2$ , which is defined as the Thermal Average of the matrix-generalized overlap ( $\text{Tr}[\mathbf{R}^2]$ ),

$$\bar{Q}^2 := \langle \text{Tr}[\mathbf{R}^2] \rangle_s^\beta \quad (9)$$

where  $\mathbf{R}^2$  can be thought of as a Hamiltonian for the Quality-Squared ( $\mathbf{H}_{\bar{Q}^2} = \mathbf{R}^\top \mathbf{R}$ ).

In Eqn. 9, the so-called *Teacher (T)* is the NN model under consideration, and  $\mathbf{R} := \frac{1}{N} \mathbf{S}^\top \mathbf{T}$  denotes the ST overlap operator between the Teacher layer weight matrix  $\mathbf{T}$  and a similar *Student (S)* layer weight matrix  $\mathbf{S}$ . The notation  $\langle \dots \rangle_s^\beta$  denotes a Thermal Average over all Student weight matrices  $\mathbf{S}$  that resemble the Teacher weight matrix  $\mathbf{T}$ . By “resemble”, the SETOL approach assumes that the ESD of  $\mathbf{S}$  has the same *limiting* form as  $\mathbf{T}$ , placing them in the same HTSR Universality class. This is made more precise below.



655 **The Overlap  $\mathbf{R}$ , and the Inner and Outer forms of  $\mathbf{A}$ ,  $\mathbf{A}_M$  and  $\mathbf{A}_N$ , resp.** Let us now  
 656 express the average matrix-matrix overlap  $\mathbf{R}$  in squared form using:

$$\begin{aligned}\text{Tr}[\mathbf{R}^2] &:= \text{Tr}[\mathbf{R}^\top \mathbf{R}] \\ &= \frac{1}{N^2} \text{Tr}[\mathbf{T}^\top \mathbf{S} \mathbf{S}^\top \mathbf{T}] = \frac{1}{N} \text{Tr}[\mathbf{T}^\top \mathbf{A}_N \mathbf{T}]\end{aligned}\tag{10}$$

657 where  $\mathbf{A}_N$  is called the *Outer* Student correlation matrix, and is the  $N \times N$  form of the Student  
 658 correlation matrix,  $\mathbf{A}_N := \frac{1}{N} \mathbf{S} \mathbf{S}^\top$ . We will also define the  $M \times M$  *Inner* Student correlation  
 659 matrix  $\mathbf{A}_M = \frac{1}{N} \mathbf{S}^\top \mathbf{S}$ , which is used later. Note that  $\mathbf{A}_M$  also has a  $\frac{1}{N}$  factor, so that its non-zero  
 660 eigenvalues will be the same as  $\mathbf{A}_N$ , but it has dimensions  $M \times M$ . We will denote the Outer  $\mathbf{A}_N$   
 661 and Inner  $\mathbf{A}_M$  forms when the context demands it, and will simply use the general form  $\mathbf{A}$  when  
 662 they can be interchanged.

663 **The Quality-Squared Generating Function  $\beta \Gamma_{\bar{Q}^2}^{IZ}$ .** As explained in Section 4.2, this Quality-  
 664 Squared is more readily obtained as the derivative of the Layer Quality-Squared Generating  
 665 Function,  $\beta \Gamma_{\bar{Q}^2}^{IZ}$ , defined as

$$\bar{Q}^2 := \frac{1}{\beta} \frac{\partial}{\partial n} \lim_{N \gg 1} \beta \Gamma_{\bar{Q}^2}^{IZ}\tag{11}$$

666 where  $n$  is the number of training examples used to train the model.

667  $\beta \Gamma_{\bar{Q}^2}^{IZ}$  is essentially ( $\beta$  times) a *negative Free Energy* for the (approximate) Layer Quality-  
 668 Squared (see Section 4, and the Appendix, Section A.3). For more details, see Section 5, and the  
 669 Appendix, Section A.2).

670 We can write  $\beta \Gamma_{\bar{Q}^2}^{IZ}$  as an HCIZ Integral,

$$\beta \Gamma_{\bar{Q}^2}^{IZ} = \frac{1}{N} \ln \int d\mu(\mathbf{S}) \exp\left(n\beta N \text{Tr}\left[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}\right]\right),\tag{12}$$

671 where  $n$  is the number of training examples used to train the models.

672 The SETOL approach then seeks to express  $\beta \Gamma_{\bar{Q}^2}^{IZ}$  in Eqn. 12 as an HCIZ integral (and in the  
 673 Wide Layer Large- $\mathcal{N}$  limit in  $N$ ) [73, 83, 84]. We evaluate this at large- $N$  in  $N$ , and write

$$\beta \Gamma_{\bar{Q}^2, N \gg 1}^{IZ} := \lim_{N \gg 1} \beta \Gamma_{\bar{Q}^2}^{IZ}\tag{13}$$

674 The result is effectively expressed in the limit of fixed *layer load*  $n/N$ , analogous to a renormal-  
 675 ized mean-field (i.e., Semi-Empirical) theory over  $N$  interacting (feature) vectors of length  $M$ .  
 676 In other words, in taking the Large- $\mathcal{N}$  in  $N$  limit, we assume implicitly that  $\beta \Gamma_{\bar{Q}^2}^{IZ}$  is in the  
 677 Thermodynamic limit (and at high-T).

678 With these definitions in place, moving forward, the following key assumptions, which can be  
 679 tested empirically, must hold:

- 680 • **The Effective Correlation Space (ECS) Condition.** The generalizing components of  
 681 the Student (and Teacher) layer weight matrices concentrate into a lower rank subspace—  
 682 the ECS—spanned by the eigenvectors associated with the (heavy) tail of the layer ESD  
 683  $\rho_{tail}(\lambda)$ , such that the test error can be reproduced with only these components. We write  
 684  $\tilde{\mathbf{A}}$  to denote the projection of the correlation matrix  $\tilde{\mathbf{A}} := \mathbf{P}_{ecs} \mathbf{A}$ , onto this subspace, now  
 685 with rank  $\tilde{M} \ll M$ . This restricts the measure  $d\mu(\mathbf{A})$  to the ECS, ( $d\mu(\mathbf{A}) \rightarrow d\mu(\tilde{\mathbf{A}})$ ). This  
 686 assumption will be empirically examined using real-world Teacher weight matrices  $\mathbf{T} = \mathbf{W}$   
 687 in Section 6.2.

688 • **The ERG Condition.** The Effective Student correlation matrix  $\tilde{\mathbf{A}}$  satisfies the **ERG** condition  
 689 that  $\text{Tr}[\ln \tilde{\mathbf{A}}] = \ln \det(\tilde{\mathbf{A}}) = 0$ , so that the change of measure  $d\mu(\mathbf{S}) \rightarrow d\mu(\tilde{\mathbf{A}})$  is Volume  
 690 Preserving. This condition is derived explicitly in terms of Inner form,  $\tilde{\mathbf{A}}_{\text{M}}$ , and will also  
 691 hold for the Outer form,  $\tilde{\mathbf{A}}_{\text{N}}$ . Practically, this implies that the  $\tilde{M}$  eigenvalues  $\tilde{\lambda}$  of the tail  
 692 of the ESD must satisfy  $\sum_{i=1}^{\tilde{M}} \ln \tilde{\lambda}_i \approx 0$ . Experiments will test this assumption explicitly in  
 693 Section 6.3.

694 Remarkably, both conditions hold best empirically when the HTSR PL quality metric  $\alpha \gtrsim 2$  is  
 695 Ideal. Motivated from these empirical observations, we have:

696 •  $\beta \Gamma_{\tilde{Q}^2, N \gg 1}^{IZ}$  is expressed as an **HCIZ** integral, at large- $N$ . We have

$$\beta \Gamma_{\tilde{Q}^2, N \gg 1}^{IZ} = \lim_{N \gg 1} \frac{1}{N} \ln \int d\mu(\tilde{\mathbf{A}}) \exp(n\beta \text{Tr}[\mathbf{T}^\top \tilde{\mathbf{A}}_{\text{N}} \mathbf{T}]) \quad (14)$$

697 where measure  $d\mu(\tilde{\mathbf{A}})$  lets us average over all (Outer) Student Correlation matrices  $\tilde{\mathbf{A}}_{\text{N}}$   
 698 explicitly, which lie in the ECS space and which “resemble” the Teacher. By “resemble” we  
 699 mean that they share the same functional form in their limiting ESDs,  $\rho_{\tilde{\mathbf{A}}}^\infty(\lambda) \sim \rho_{\tilde{\mathbf{X}}}^\infty(\lambda)$ .

700 • **The Layer Quality (Squared)  $\tilde{Q}^2$  is a Norm Generating Function.** The final ex-  
 701 pression for  $\tilde{Q}^2$  can be written as the derivative of  $\beta \Gamma_{\tilde{Q}^2, N \gg 1}^{IZ}$  as

$$\tilde{Q}^2 = \frac{1}{\beta} \frac{\partial}{\partial n} \beta \Gamma_{\tilde{Q}^2, N \gg 1}^{IZ} = \sum_{i=1}^{\tilde{M}} \mathcal{G}(\lambda_i) \quad (15)$$

702 where  $\mathcal{G}(\lambda_i)$  is, albeit imprecisely, a *Norm Generating Function*, and is defined as the  
 703 integrated *R-transform*  $R(z)$  of the Teacher layer ESD (where  $z \in \mathbb{C}$ ), such that  $\mathcal{G}(\lambda) :=$   
 704  $\int_{\tilde{\lambda}_{\min}}^{\lambda} R(z) dz$  and  $\tilde{\lambda}_{\min}$  encapsulates the ECS (and, for some choices of  $R(z)$ , selects the  
 705 desired branch-cut of  $R(z)$  so that it is both analytic and well-behaved).

706 To apply the theory, one must choose an R-transform  $R(z)$  for the Teacher that models the  
 707 tail of the ESD  $\rho_T^{\text{emp}}(\lambda)$ , and that can be parameterized by some measurable property. This may  
 708 include the number of Spikes  $\lambda^{\text{spike}}$ , the fitted PL exponent  $\alpha$ , the maximum eigenvalue  $\lambda_{\max}$ ,  
 709 or even the entire tail  $\rho_T^{\text{tail}}(\lambda)$ . This may be a formal expression, a computational procedure, or  
 710 some combination.

711 To integrate  $R(z)$ , however, and to have a physically meaningful result, one must ensure that  
 712  $R(z)$  is both analytic and single-valued on the domain of interest, namely, the ECS (and therefore  
 713 the (PL) tail of the ESD),  $\Re[z] \geq \tilde{\lambda}_{\min}$ .<sup>13</sup> Because the ESD is frequently Heavy-Tailed (HT), this  
 714 R-transform  $R(z)$  may have a branch-cut, and it is expected that this will occur at  $\Re[z] \approx \tilde{\lambda}_{\min}$ ,  
 715 corresponding to a point roughly at or before the start of the ECS (i.e., at the peak of the ESD on  
 716 a log scale). Selecting the branch-cut  $R(z)$  provides an additional physical meaning to the ECS.

717 To complete the theory, we will also show that the HTSR PL Layer Quality metrics **Alpha**  
 718 ( $\alpha$ ) and **AlphaHat** ( $\hat{\alpha}$ ) can be formally derived directly from the **SETOL** Layer Quality  $\tilde{Q}$  by  
 719 selecting the appropriate R-transform  $R(z)$  and making empirically motivated approximations.  
 720 In Section 5.4 we provide several possible models of  $R(z)$  and the resulting Layer Quality  $\tilde{Q}$ .

721 **Renormalization Group Effective Hamiltonian** The formulation of SETOL closely paral-  
 722 lels the construction of an Effective Hamiltonian  $\mathbf{H}_{\tilde{Q}^2}^{\text{ECS}}$  via the Wilson Exact Renormalization

<sup>13</sup> $\Re[z]$  is the Real part of  $z$ .

Group (ERG) approach. Consider a *bare* Hamiltonian  $\mathbf{H}_{\bar{\mathcal{Q}}^2}$  for the Layer Quality-Squared, defined as  $\mathbf{H}_{\bar{\mathcal{Q}}^2} := \mathbf{R}^\top \mathbf{R}$ . We can express Eqn. 12 in terms of this bare Hamiltonian  $\mathbf{H}_{\bar{\mathcal{Q}}^2}$ , and rewrite Eqn. 14 in terms of a *Renormalized* Effective Hamiltonian  $\mathbf{H}_{\bar{\mathcal{Q}}^2}^{ECS}$  that spans the Effective Correlation Space (ECS). Formally, we have:

$$\frac{1}{N} \ln \int d\mu(\mathbf{S}) e^{n\beta N \text{Tr}[\mathbf{H}_{\bar{\mathcal{Q}}^2}]} \xrightarrow{ERG} \lim_{N \gg 1} \frac{1}{N} \ln \int d\mu(\tilde{\mathbf{A}}) e^{n\beta N \text{Tr}[\mathbf{H}_{\bar{\mathcal{Q}}^2}^{ECS}]} \quad (16)$$

where the ERG transformation is defined by the Scale-Invariant change of measure, applied in the Wide Layer Large- $\mathcal{N}$  limit in  $N$ , and where  $\mathbf{H}_{\bar{\mathcal{Q}}^2}^{ECS}$  is defined implicitly through the result for  $\bar{\mathcal{Q}}^2$  (Eqn. 15). The result is, formally, a sum of the integrated R-transforms  $\mathcal{G}(\lambda_i)$ . In a sense, this result resembles (a non-perturbative form of) the Linked Cluster Theorem in that the log Partition Function is expressed as a sum of integrated matrix-generalized cumulants. And in analogy with Semi-Empirical theories of Quantum Chemistry, the HTSR Alpha ( $\alpha$ ) and AlphaHat ( $\hat{\alpha}$ ) enter as renormalized empirical parameters. Most importantly, the Scale-Invariant ERG condition can be verified empirically (See Section 6.) Importantly, in analogy with the Wilson Exact Renormalization Group theory, the HTSR  $\alpha = 2$  resembles in spirit an ERG *Universal Critical Exponent* at a phase boundary being between the Heavy-Tailed (HT) and the Very Heavy-Tailed (VHT) phase of learning of the HTSR theory. This observation strengthens our argument that the HTSR HT and VHT phases are analogous to the generalizing and overfitting phases, respectively, of the classical SMOG theories of NN learning.

### 3.2 Comparing SETOL with HTSR: Conditions for Ideal Learning

The SETOL approach establishes a starting point for developing a first-principles theory for modern NNs. Among other things, by connecting with the HTSR phenomenology, it lets us identify conditions for an Ideal state of learning for an individual NN layer, under the Single Layer Approximation. By Ideal, we mean that the layer is being used most effectively i.e., in some sense it is at its optimal data load, and thus it is conjectured to result in the best model quality.

**The Ideal State of Learning** is conjectured to be characterized by the following three conditions:

1. the tail of ESD,  $\rho_{tail}^{emp}(\lambda)$ , can be well fit to a PL of  $\alpha \approx 2$ :  $\rho_{tail}^{emp}(\lambda) \sim \lambda^{-2}$ ;
2. the eigenvalues in the tail,  $\lambda_i$ , satisfy the ERG (i.e., Trace-Log) condition:  $\sum_i \ln \lambda_i = 0$ ; and
3. the generalizing components of the layer concentrate in the singular vectors associated with the tail of the ESD, (whose span we call the Effective Correlation Space).

In Section 6, we will test and justify this conjecture by showing that the induced measures of each condition converge to one another at the same rate, and reach convergence at the exact point beyond which accuracy begins to degrade.

These claims are fundamentally about NN learning itself. They are motivated by our formulation of the SETOL approach in our search for a practical predictive theory behind the HTSR phenomenology. When (1) and (2) conditions hold for any layer, we conjecture that (3) holds as well. Moreover, when (1–3) hold for all layers, we conjecture the NN has the lowest Generalization Error (and highest Model Quality) possible for given model architecture and dataset.

Previous results have shown that the HTSR quality metrics (Alpha, AlphaHat, etc.) correlate very well with reported test accuracies, as well as model quality on an epoch-by-epoch basis [25, 85]. These results hold because, as indicated by the HTSR theory, the PL exponent  $\alpha$  characterizes both the quality of the layer and provides an after-the-fact measure of the amount of

regularization.<sup>14</sup> However, the HTSR approach says nothing about the SETOL ERG condition; and neither does the SETOL approach require a minimum of  $\alpha = 2$  to obtain the best model quality, as observed by the HTSR phenomenology. Remarkably, we can show that (1) and (2) do hold *simultaneously*, both in carefully designed experiments on a small model, as well as for many pre-trained, high quality open-source models (such as VGG, ResNet, Llama, Falcon, etc).

HTSR, however, has been developed as a phenomenology describing the best-trained, most accurate open-source models available. As such, it may be biased towards such models, and it may not describe less optimal learning scenarios. The key goal of this work is to derive independent conditions, both theoretical and experimental, that can identify the conditions for Ideal Learning, and to stress-test these conditions in carefully designed, reproducible experiments.

### 3.3 Detecting Non-Ideal Learning Conditions

The HTSR phenomenology posits that SGD training reduces the *Training Error* by accumulating correlations into the large eigenvalues in NN layer weight matrices  $\mathbf{W}$  such that they *self-organize* into a HT with a PL signature, and that this successful self-organization leads to good model quality. Conversely, it also posits that when training has gone awry in some way, the resulting ESD,  $\rho^{emp}(\lambda)$ , will be deformed in some way. In many practical situations, there can be other, competing factors that give rise to large eigenvalues that do not contribute to the generalization capacity of the model, and, consequently, can affect the Scale (i.e., the largest eigenvalue(s)  $\lambda_{max}$ ) and Shape (i.e., the PL exponent  $\alpha$ , or goodness of fit  $D_{KS}$ ) of the layer ESDs. These large  $\lambda$  could be Dragon Kings [86], *Correlation Traps*, or some other anomaly.

To apply the HTSR phenomenology most effectively, one must be able to identify various spurious factors and distinguish real correlations from any other large eigenvalues, including the effects of both extreme eigenvalues  $\lambda$ , individual matrix elements  $W_{i,j}$ , and rank-1 perturbations in  $\mathbf{W}$ . In one case the ESD is HT primarily due to correlations that help the model generalize, whereas in another when the ESD may be more HT than expected due to suboptimal training, mis-labeled data, etc. In extreme cases, spurious eigenvalues can push the weight matrix into the Very Heavy-Tailed Universality class (i.e.,  $\alpha < 2$ . See Table 1, Section 2), or disrupt the formation of a HT, resulting in a poor PL fit, undermining the core proposition of the HTSR approach.

When training a model with SGD, one may only achieve a sub-optimal result when using overly large learning rates / small batch sizes, (see Section 6), from poor hyper-parameter settings, or simply because direct regularization fails. In such cases, the HTSR approach allows one to detect potential problems by looking for large eigenvalues *not* resulting from correlations [87].

Importantly, in the context of the SETOL theory, we can now identify such empirical anomalies due to atypical layer weight matrices  $\mathbf{W}$ , a key factor when models break down. The SETOL approach formalizes the empirical HTSR phenomenology, but, in doing so, assumes that the underlying layer effective correlation matrix  $\tilde{\mathbf{X}}$ , is typical, meaning that it can describe out-of-sample / test data. Conversely, if the underlying weight matrix  $\mathbf{W}$  is atypical, then it is in some sense overfit to the training data and can not fully represent out-of-sample / test data. Consequently, when  $\mathbf{W}$  is atypical, we argue that we can observe this, either in the ESD  $\rho^{emp}(\lambda)$  directly (i.e., when  $\alpha < 2$ ), and/or having 1 or more unusually large matrix elements  $W_{ij}$ .

We conjecture such sub-optimal results, and particularly those occurring from overfitting, actually arise when the underlying layer weight matrix  $\mathbf{W}$  is atypical in some way, in analogy to

<sup>14</sup>By “after-the-fact”, we mean that it provides a measure of the regularization in a layer, along the lines of the self-regularization interpretation of HTSR Theory [25]. However, we do *not* recommend that it be used as an explicit regularization parameter. Informally, this is since the “easiest way to obtain HT ESDs is to make weight matrices HT element-wise; but this is *not* what is observed in practice, and thus this is precisely *not* what HTSR Theory and our new SETOL approach are designed to model.

the results from the classic SMOG theory (see Section 4.1), and, importantly, that we can use the SETOL approach to detect when  $\mathbf{W}$  is atypical and therefore a layer is overfit in some way.

Here, we identify two specific cases of atypical weight matrices—Correlation Traps and *Over-Regularization*.<sup>15</sup>

**3.3.1 Correlation Traps.**  $\mathbf{W}$  is atypical in that  $\mathbf{W}$  exhibits an anomalously large mean ( $\bar{\mathbf{W}}$ ). We can observe these by randomizing the layer weight matrix,  $\mathbf{W} \rightarrow \mathbf{W}^{rand}$ , and then looking for eigenvalues that extend significantly beyond the MP edge of the random bulk (i.e., Spikes). We call such random spikes *Correlation Traps*, denoted as  $\lambda_{trap}$ , because they appear, in some extreme cases, to be associated with distorted ESDs and, importantly, lower test accuracies. Examples of Correlation Traps are shown in Section 6.5.

**3.3.2 Over-Regularization.**  $\mathbf{W}$  is atypical in that  $\mathbf{W}$  exhibits an anomalously large variance ( $\sigma^2(\mathbf{W})$ ). We can observe this when the layer  $\alpha < 2$ . Also, since Alpha a measure of implicit regularization, we say the layer with  $\alpha < 2$  is *Over-Regularized*. In particular, when one layer is undertrained, having  $\alpha > 6$ , it appears that other layers may become overtrained to compensate, and this can be seen with having  $\alpha < 2$ . These effects are studied in Section 6. Additionally, we also observe that when evaluating the SETOL ERG condition, when  $\alpha < 2$ , then  $\Delta\lambda_{min} < 0$  (see Section 6.3).

### 3.3.1 Correlation Traps

The first way we identify  $\mathbf{W}$  as atypical is when it has an anomalously large mean ( $\bar{\mathbf{W}}$ ); detecting this in general, however, requires more than just examining which elements  $W_{i,j}$  are anomalously large but, instead, looking for what can be multi-element rank-1 perturbations in  $\mathbf{W}$ . Here, we can apply elementary RMT, as in the HTSR approach.

The HTSR phenomenology states that NNs generalize better when their layers ESDs are more HT—precisely because the tail eigenvalues arise from correlations in the weight matrices. So one way is to identify *atypicality* is to look for large eigenvalues that do not arise from correlations in  $\mathbf{X}$ , but, rather, from one or a few spuriously large matrix elements  $W_{i,j}$  and/or rank-1 perturbations in  $\mathbf{W}$ . We call these eigenvalues Correlation Traps, denoted by  $\lambda_{trap}$  (i.e., see Section 6.5).

Indeed, if we randomize  $\mathbf{W}$  element-wise, i.e  $\mathbf{W} \rightarrow \mathbf{W}^{rand}$ , we expect the  $W_{i,j}^{rand}$  matrix elements to be i.i.d and with a small mean (unless something odd happens during SGD training). Likewise, we expect the singular values of  $\mathbf{W}^{rand}$  to follow the MP distribution, to within finite-size / TW fluctuations. If we observe an eigenvalue  $\lambda_{trap}$  extending beyond the MP bulk region,  $\lambda_{trap} > \lambda_{bulk}^+$ , then the mean  $W_{i,j}$  matrix element will also be anomalously large, and we can identify  $\mathbf{W}$  as atypical. We must be careful, however, as we do not fully understand the origin of these atypicalities and do not claim that every one is associated with suboptimal generalization.

By a *Correlation Trap*, we mean that some anomaly in the training of  $\mathbf{W}$  resulted in one or more spuriously large eigenvalues  $\lambda_{trap}$  in  $\mathbf{W}^{rand}$ , and that whatever caused them also may, in some pronounced cases, tend to “trap the correlations in  $\mathbf{X}$  itself, preventing them from coalescing into a well defined PL Heavy Tail, or otherwise distorting the ESD. Whether they are a signature of training gone wrong, or whether they distort the dynamics of the tail correlations simply by being there, Correlation Traps can be expected to alter the shape of the ESD, reducing the quality of the PL fits, and sometimes producing spurious  $\alpha$  values.

Why would such anomalies occur in a NN? It is conceivable that SGD will, when it fails to find usable correlations, instead produce spurious correlations in the form of large elements

<sup>15</sup>Later, in Section 6, we will show that we can systematically induce both phenomena and observe their effects on the HTSR HT PL metric  $\alpha$  and the SETOL ERG condition.



and/or rank-1 perturbations. Also, the matrix itself may simply undergo an innocuous mean-shift because the mean is not explicitly controlled during training. Here, mean-recentering may be beneficial.<sup>16</sup>

We will see, below in Section 6, that we can induce a Correlation Trap both by shrinking the batch size, or, equivalently, increasing the learning rate, and that this is associated with degraded model performance and small  $\alpha$ . We seek to identify specific ways of identifying such traps because we reason that the presence of foreign large eigenvalues may disrupt the self-organization of correlations – or that failed learning may produce them as a by-product.

**Detecting Correlation Traps with RMT.** RMT suggests that when a matrix  $\mathbf{W}$  has unusually large elements  $W_{ij}$ , then the ESD will have one or more large eigenvalues  $\lambda_{trap}$  lying outside the bulk edge  $\lambda_{bulk}^+$  of the ESD, as predicted by MP theory. One can detect these so-called Correlation Traps in a weight matrix  $\mathbf{W}$  by performing the following:

1. randomize  $\mathbf{W}$  element-wise to obtain  $\mathbf{W}^{rand}$ ;
2. compute the ESD for  $\mathbf{W}^{rand}$ ; and
3. look for large eigenvalues  $\lambda_{trap} \gg \lambda_{bulk}^+$ .

**WeightWatcher** looks for Correlation Traps ( $\lambda_{trap}$ ) in the ESD of the randomized  $\mathbf{W}^{rand}$ , that are larger than  $\lambda_{trap} > \lambda_{bulk}^+ + \Delta_{TW}$ , where  $\lambda_{bulk}^+$  is the MP bulk edge  $\Delta_{TW}$  are the associated finite-size Tracy Widom (TW) fluctuations. This procedure detects *any* anomaly in the matrix weights that produce spuriously large eigenvalues. It is implemented in **WeightWatcher** (using the randomize option), which was used to generate the plots in Figure 5.

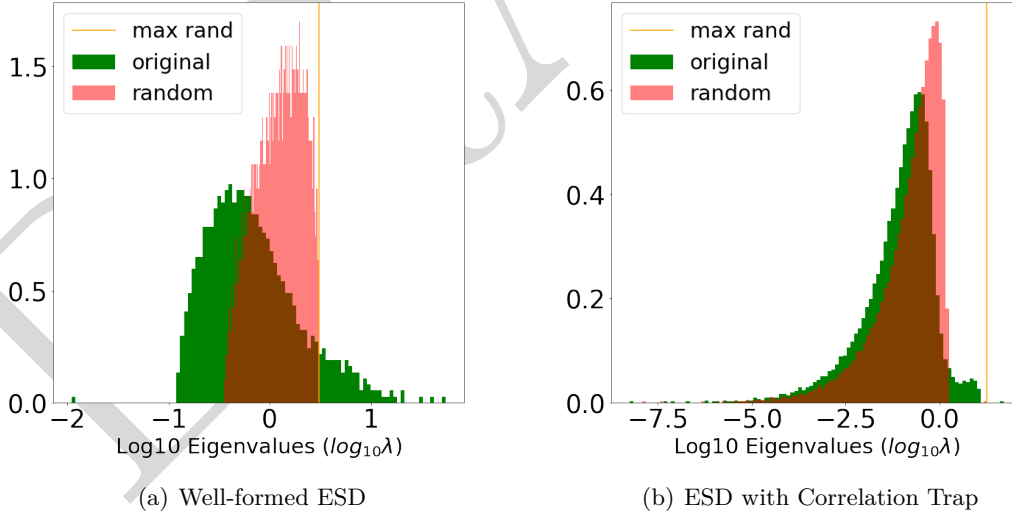


Figure 5: Comparison of a well-formed, Heavy-Tailed ESD (a) to one with a Correlation Trap (b), in the VGG16 model (FC2 layer)

See Figure 5(a), which displays the (log)-ESD of a typical SOTA NN layer  $\mathbf{X}$  (green), i.e., on a log-linear scale, along with the (log)-ESD of that layer after randomizing it element-wise (red).

<sup>16</sup>Similarly, when training NNs, frequently the weight matrices [88] or activations [89] may need to be clipped during training to ensure good results.



The two ESDs differ substantially: the ESD of the original weight matrix  $\mathbf{W}$  (green) is very HT, whereas the ESD of the randomized weight matrix  $\mathbf{W}^{rand}$  (red) is an MP (and as predicted by the MP RMT). The orange line corresponds to the maximum eigenvalue of the randomized ESD. Note that it is at the MP bulk edge of the red plot, indicating that this ESD is not affected by unusually large elements or other weight anomalies. Here, we say that the ESD of  $\mathbf{X}$  is HT, and that  $\mathbf{W}$  is not HT element-wise. HTSR says this layer is well trained.

Contrast this with Figure 5(b), which displays the (log)-ESD of a NN layer with a Correlation Trap. The ESD of  $\mathbf{X}$  (green) is weakly HT, but it looks nothing like the ESD in Figure 5(a). In fact, it looks very much like the ESD of the randomized weight matrix  $\mathbf{W}^{rand}$  (red), except for a small shelf on the right. The orange line again corresponds to the maximum eigenvalue of the randomized ESD, and this is just past this shelf. Relative to the randomized ESD, this line depicts (an) unusually large element(s)—or, equivalently, a rank-1 perturbation of  $\mathbf{W}^{rand}$ . By a Correlation Trap, we mean that some anomaly in the elements of  $\mathbf{W}$  tends to “trap” the ESD of  $\mathbf{X}$ , concentrating the correlations in  $\mathbf{X}$  into the small shelf of density around the orange line. HTSR says this layer is not well-trained because it does not have a good PL fit.

### 3.3.2 Over-Regularization

The second way we identify  $\mathbf{W}$  as atypical is when it has an anomalously large variance ( $\sigma^2(\mathbf{W})$ ).

The SETOL theory – a single-layer theory of learning – casts the training of a NN layer in terms of how the correlations concentrate into the layer Effective Correlation Space (ECS), and becomes exact when the ERG condition is satisfied. Analogously, the HTSR theory – a single layer phenomenology of learning – casts training of an N layer by fitting its ESD to a PL, and noting that the PL exponent  $\alpha$  measures the amount of implicit regularization in the layer. Comparing the two approaches, we see that smaller  $\alpha$  corresponds to the correlations concentrating into a low-rank ECS. In general, and likewise, the more the weight matrix correlations concentrate into a low-rank ECS, the better the layer has been regularized. A natural question arises then, namely, can a layer be *Over-Regularized* and can we detect this? and in large, Empirically, we do indeed observe that over the course of training,  $\alpha$  decreases, (See Figure 27 (a), Section 6.6,) and that the models predictions are concentrated into the ECS, (See Section 6.2). Thus, we also interpret  $\alpha$  and ECS concentration to be measures of learning itself, meaning that NNs are self-regularizing [25].

Importantly, however, the HTSR phenomenology indicates that Alpha usually lies in the Fat-Tailed Universality class, such that  $\alpha \in [2, 6]$ . When  $\alpha < 2$ , the ESD is Very Heavy Tailed (VHT), and, also, this indicates that  $\mathbf{W}$  has an anomalously large variance. That is,  $\mathbf{W}$  is atypical. Occasionally, but very infrequently, we do observe  $\alpha < 2$ , and in large, production quality models (like Llama). Interestingly, we also observe that, frequently, when the HTSR  $\alpha < 2$ , the SETOL ERG condition holds fairly well. This is further explored in Section 6

We have applied the **WeightWatcher** tool to have examined dozens of modern, very large NNs; of particular interest are the so-called Large Language Models (LLMs) that have revolutionized the field of AI. To that end, in Figure. 6, we present the **WeightWatcher** layer Alpha metrics for the Falcon-40b and the Llama-65b LLMs. <sup>17</sup>

For the Falcon-40b model, all of the layer Alpha range between  $\alpha \in [2, 6]$ , and therefore lie in the Fat-Tailed Universality class (in Table 1) and are well-fit. In contrast, looking at the Llama-40b layer Alpha, very many have  $\alpha > 6$ , indicating these layers are under-fit, and while a few have  $\alpha < 2$ , suggesting these are over-fit. Finally, there are more layers with  $\alpha \sim 2$  in Llama-65 vs Falcon-40b.

<sup>17</sup>Similar results are found for the larger, more modern Llama models, and can be found on the **WeightWatcher** website[67]

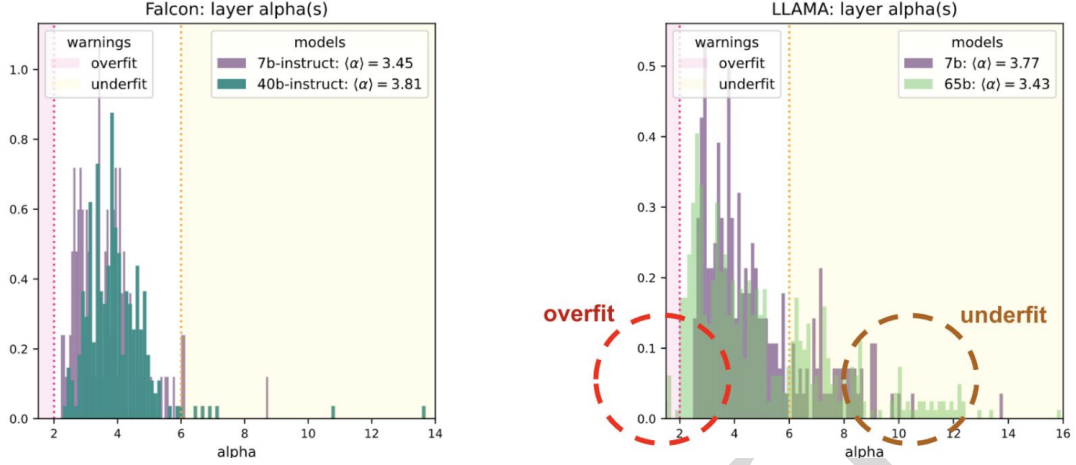


Figure 6: Falcon vs Llama

The observations on Llama-2 suggest that the layers with  $\alpha \leq 2$  are compensating for the layers with  $\alpha > 6$ , and yielding suboptimal performance for the Llama-65b architecture. Based on these observations, we hypothesize that, in a multi-layer-perceptron (MLP), when one layer does not or can not learn, then other layers will have to compensate, and will be overloaded with the training data, leading to  $\alpha < 2$ , and even the **ERG** condition  $\Delta\lambda_{min} < 0$ .

In Section 6.6, we will test this hypothesis. By reducing the trainable parameters in a small MLP, we can simulate the situation seen above in the Llama-65b model, and observe the formation of a Very Heavy Tailed (VHT) ESD in the dominating layer weight matrix. Overloading results from having too few parameters for the complexity of the task. Adding more data increases the load up to the total complexity of the task itself.

Moreover, we will also argue that in our experiments, the model enters a kind of glassy meta-stable phase, similar to the kinds of phases predicted by classic **StatMech** theories of learning [8] (described below). Section 6.6 will explore how far we can push the analogy of glassy systems in our experiments to stress test the **SETOL** approach. In particular, we will see effects such as the slowing down of its dynamics, leading to a kind of hysteresis, specific to the under-parameterized regime.

## 4 Statistical Mechanics of Generalization (SMOG)

In this section, we review the **StatMech** approach to learning: both to understand how it is usually applied in Statistical Mechanics of Generalization (SMOG) theory; and to understand how our Semi-Empirical approach in SETOL is similar to and different from the traditional approach. We will also obtain an expression for the Generalization Accuracy (or Model Quality  $\bar{Q}^{ST}$ ) for the classic Student-Teacher (ST) model of the Linear Perceptron (in the AA, and at high-T), as described in [7, 8]. In Section 5, we will generalize this to a Layer Quality metric,  $\bar{Q}$ , for a layer in a general Multi-Layer Perceptron (MLP), i.e.,  $\bar{Q}^{ST} \rightarrow \bar{Q}$ , so that  $\bar{Q}$  can then be expressed in terms of the ESD of the NN layer.

**Outline.** Here is an outline of this section.

- **Approaches to the SMOG.** In Section 4.1, we explain the mapping from the **StatMech** theory of disordered systems to the **StatMech** theory of NN learning (SMOG); and how our Semi-Empirical approach (SETOL) is similar to and different from the traditional approach.
- **Mathematical Preliminaries.** In Section 4.2, we review the mathematical details of **StatMech**, providing definitions and detailed derivations of quantities and expressions necessary later.
- **Student-Teacher Model.** In Section 4.3, we discuss the setup of the Student-Teacher (ST) model as a general means to estimate the Average Generalization Error empirically. First, in subsection 4.3.1, we describe the ST setup with an operational analogy. Then, in subsection 4.3.2, we derive the (new) result for the ST Model Quality,  $\bar{Q}^{ST}$ , using the setup of the classic (ST) model for the Generalization Error (and accuracy) of the Perceptron (in the AA, and at high-T).

Additional information can be found in the Appendix.

- **Symbols and Equations.** In Section A.1, we summarize the important symbols and key results, including the dimensions of the vectors and matrices, different notations for energies, and key equations.
- **Summary of the SMOG.** In Section A.2, we provide a more detailed analysis of the results we derive in Section 4.3.2. In particular, in Section A.2.1, we repeat the derivations of the ST Generalization Error  $\bar{\mathcal{E}}_{gen}^{ST}$  and related quantities (from Section 4.2), using more concrete notation to align with [7, 8]; and in Section A.2.2, we use this to derive the matrix-generalization of the ST Annealed Error Potential  $\epsilon(R)$  (as well as the normalization for the weight matrices, necessary for later).

### 4.1 StatMech: the SMOG approach and the SETOL approach

In this subsection, we review the basic **StatMech** setup necessary to understand SMOG theory as well as SETOL. This theory was developed in the 1980s and 1990s [7, 8, 90, 6, 91, 5].

**Traditional SMOG theory.** In traditional SMOG theory, one maps the learning process of a NN to the states and energies of a physical system. The mapping is given in Table 2. SMOG theory models the SGD training of a *Perceptron* on the data,  $\mathbf{x}^n$ , to learn the optimal weights,  $\mathbf{w}$ , as a Langevin process.<sup>18</sup> The power of the **StatMech** approach comes from the fact that the core

<sup>18</sup>Typically, we have no guarantee of the true equilibrium in a high-dim nonconvex landscape; so, when the *Thermodynamic limit* exists, the Langevin process converges or relaxes to the thermodynamic equilibrium.

Statistical Physics	Neural Network Learning
Gaussian field variables	Gaussian i.i.d (idealized) data $\xi^n \in \mathcal{D}$
State Configuration	Trained / Learned weights $\mathbf{w}$
State Energy Difference	Training and Generalization Errors $\bar{\mathcal{E}}_{train}, \bar{\mathcal{E}}_{gen}$
Temperature	Amount of regularization present during training $T$
Annealed Approximation	Average over data $\xi^n$ first, then weights $\mathbf{w}$ .
Thermal Average	Expectation w.r.t. the distribution of trained models
Free Energy	Generating function for the error(s) $F$

Table 2: Mapping between states and energies of a physical system and parameters of the learning process of a neural network.

SETOL Terminology	Explanation
Model Quality $\bar{Q}$	Generalization accuracy, in the AA and at high-T
Layer Quality $\bar{Q}$	Layer contribution to the accuracy, in the AA and at high-T
Layer Quality-Squared $\bar{Q}^2$	Layer Quality squared, used for technical reasons
Quality Generating Function $\Gamma_{\bar{Q}}, \Gamma_{\bar{Q}^2}$	Generating function for Quality
Annealed Hamiltonian $H^{an}$	Energy function, for errors or accuracies
Effective Hamiltonian $H^{eff}$	Exact energy function, but restricted to a low-rank subspace

Table 3: Additional terminology introduced for the SETOL. Notice that the Quality Generating Function  $\Gamma$  is simply one minus the Free Energy,  $\Gamma := 1 - F$ , but it is introduced because sign convention for the Free Energy is always decreasing with the error. In contrast, we define the Hamiltonian in terms of the model error or accuracy, depending on the context.

concept of Thermal average corresponds to taking the expectation of a given quantity only *over the set of trained models*, as opposed to uniformly over all possible models (or in a worst-case sense, over all possible models in a model class). This capability is particularly compelling in light of the StatMech capacity to characterize disordered systems with complex non-convex energy landscape (which can even be *glassy*, characterized by a highly non-convex landscape [8, 82, 91], and recognized classically by a slowing down of the training dynamics [92]). Thus, concepts such as training and Generalization Error arise naturally from integrals that are familiar to StatMech; and theoretical quantities such as Load, Temperature, and Free Energy also map onto useful and relevant concepts [93]. The Free Energy is of particular interest because it can be used as a generating function to obtain the desired Generalization Error and/or accuracy. We wish to understand how to compute the associated thermodynamic quantities such as the expected value of the various forms of the Average Generalization Error ( $\bar{\mathcal{E}}_{gen}$ ), Partition Function ( $Z$ ), and the Free Energy ( $F$ ) and other Generating Functions ( $\Gamma$ ).

**The Student-Teacher model.** We seek to compute and/or estimate the Average Generalization Accuracy for a *fixed* Teacher Perceptron  $T$  by averaging over an ensemble of Student  $S$  Perceptrons, in the Annealed Approximation (AA), and at High-Temperature (high-T); we call this ST Model Quality, and denote it  $\bar{Q}^{ST}$ . In Section 5, we generalize  $\bar{Q}^{ST}$  to an arbitrary

layer in a Multi-Layer Perceptron, giving a Layer Quality, i.e.,  $\bar{Q}^{ST} \rightarrow \bar{Q}$ . This formulation of the ST problem differs from the classic approach [8, 91] in that we treat the Teacher as input to the theory rather than a random vector  $\mathbf{t}$  and that Teacher provides the trained weights  $\mathbf{w}$  explicitly as opposed to the labels  $y_\mu^T$ . In the simpler Perceptron formulation, there are only a few degrees of freedom (i.e., the ST overlap  $R$ , the feature load, the inverse Temperature  $\beta$ , and the number of training examples  $n$ ), whereas in the matrix generalization, the structure of the empirical Teacher weight matrix  $\mathbf{T} = \mathbf{W}$  provides  $N \times M$  additional degrees of freedom, allowing for a much richer theoretical analysis. This is one of many ways that distinguishes the current approach from previous work. Because of this, we present both a pedagogic derivation of  $\bar{Q}^{ST}$  (for a general NN in Section 4.2, and for the ST model specifically in the Appendix, Section A.2), whereas in Section 4.3.2 we provide a simple derivation, assuming the Annealed Approximation and High-Temperature at all times.

**Towards a Semi-Empirical Theory.** In the SETOL approach to StatMech, we want a matrix generalization of the Student-Teacher Model Quality,  $\bar{Q}^{ST}$ , for a single Layer Quality  $\bar{Q} \sim \bar{Q}_L^{NN}$  in an arbitrary Multi-Layer Perceptron (MLP). This matrix generalization is a relatively straightforward extension of the classical (i.e., for a vector Teacher) SMOG ST Model Quality (but our SETOL approach will use it in a conceptually new way).

In our matrix generalization, the Teacher vector  $\mathbf{t}$  is replaced by a Teacher matrix  $\mathbf{T}$  (i.e.,  $\mathbf{t} \rightarrow \mathbf{T}$ ); and, in our SETOL approach,  $\mathbf{T}$  represents actual (pre-)trained NN weight matrix (i.e.,  $\mathbf{T} \simeq \mathbf{W}$ ) that has been trained on real-world, strongly correlated data  $\mathbf{D}$ . As such, for our SETOL theory, we seek an expression that can be parameterized by the Teacher, and in particular by the ESD of the Teacher. This is what makes the basic method Semi-Empirical: we make a modeling assumption that the Teacher has the same limiting spectral distribution as the Student, and hence the same PL fit parameter  $\alpha$ . This is all done with the understanding that later we will augment (and hopefully “correct”) our mathematical formulations with phenomenological parameters fit from experimental data. To make the Semi-Empirical method a Semi-Empirical *Theory*, we not only seek to parameterize our model; but we also try to understand how to derive HTSR empirical metrics, such as Alpha and AlphaHat, how they arise from this formalism, how they are related to the correlations in the data, and why they are transferable and exhibit Universality. Importantly, we do not just seek a method with adjustable parameters, but rather formulate the theory using techniques similar to those to explain the origins of Quantum Chemistry Semi-Empirical methods, resulting in formal expressions that resemble a renormalized Self-Energy and/or Effective Hamiltonian from such approaches [94, 54, 52, 95, 50, 51, 57]. This gives what we call a Semi-Empirical *Theory*.

## 4.2 Mathematical Preliminaries of Statistical Mechanics

**SubSection Roadmap** Briefly, in the following subsection, we start by defining an arbitrary NN model, with weights ( $\mathbf{w}$ ). Then, we explain the difference between using real-world ( $\mathbf{x}$ ) and random data ( $\xi$ ). This lets us define an energy error function,  $E_{\mathcal{L}}^n(\mathbf{w})$ , the error the NN makes on the data. We then explain how to take different kinds of *Thermodynamic* averages of the data, including *Sample* and *Thermal average* and the implications, and the difference between computing errors and accuracy. Next, we define the *Free Energy* ( $F$ ) for the error(s), and the *Generating Function* ( $\Gamma$ ) for the accuracy and/or quality. From here, we explain the *Annealed Approximation* (AA) and how to define the *Annealed Hamiltonian*,  $H^{an}(\mathbf{w})$ , a crucial expression that will be the starting point later for our matrix model. In the AA,  $H^{an}(\mathbf{w})$  simplifies to  $H_{hT}^{an} = \epsilon(\mathbf{w})$ , where  $\epsilon(\mathbf{w})$  is an Annealed Error Potential that depends only on the weights  $\mathbf{w}$ . Likewise, we can define the Self-Overlap,  $\eta(\mathbf{w}) := 1 - \epsilon(\mathbf{w})$ , which is useful for obtaining the



Quality. We show how to obtain the *Average Training and Generalization Errors*  $\bar{\mathcal{E}}_{train}, \bar{\mathcal{E}}_{gen}$  using the **StatMech** formalism, which defines them in terms of partial derivatives of the Free Energy ( $F$ ). Doing this, we show that in the AA and at high-T they are equivalent,  $[\bar{\mathcal{E}}_{train}^{ST}]^{an,hT} = [\bar{\mathcal{E}}_{gen}^{ST}]^{an,hT}$ , and can both be expressed as a Thermal Average over all Students, as a function of the Teacher, as  $[\bar{\mathcal{E}}_{gen}^{ST}]^{an,hT} = \langle H_{hT}^{an}(R) \rangle_s^\beta = \langle \epsilon(R) \rangle_s^\beta$ . Note that these averages are obtained by using the Free Energy as a Generating Function. We then explain how to obtain the Model Quality as partial derivatives of a *Generating Function* ( $\Gamma_{\bar{\mathcal{Q}}}$ ). We then discuss the more advanced techniques, the *Large- $\mathcal{N}$  Approximation* and the *Saddle Point Approximation* (SPA), which will be used extensively later. Finally, we introduce HCIZ integrals, which will be necessary to evaluate the matrix-generalized form of  $\Gamma_{\bar{\mathcal{Q}}}$  to obtain the final result.

In this subsection, we will compare and contrast several types of averages, energies and other Thermodynamic concepts we will encounter.

**4.2.1 Setup.** In Section 4.2.1, we will start by describing the basic setup of the problem, including the distinction between the actual training process and how we model the training process.

**4.2.2 BraKets, Expected Values, and Thermal Averages.** In Section 4.2.2, we will describe our use of physics BraKet notation for both Sample Averages (over the data  $\mathbf{x}$ ) and Thermal Averages (over the weights  $\mathbf{w}$ ) and—in particular, under the Annealed Approximation (AA) and in the High-Temperature (High-T) limit—showing how they relate to each other and to the notion of Replica Averages.

**4.2.3 Free Energies and Generating Functions.** In Section 4.2.3, we will make a connection between these different averaging notions and Free Energies and Generating Functions, showing how they relate to each other.

**4.2.4 The Annealed Approximation (AA) and the High-Temperature Approximation (high-T).** In Section 4.2.4, we explain the Annealed Approximation, the High-Temperature approximation, and the Thermodynamic Large- $\mathcal{N}$  limit and the Saddle Point Approximation (SPA). We also introduce the Quality Generating Function  $\Gamma_{\bar{\mathcal{Q}}}$

**4.2.5 Average Training and Generalization Errors and their Generating Functions.** In Section 4.2.5, we will show how to compute the Average Training and Test/Generalization Errors  $\bar{\mathcal{E}}_{train}, \bar{\mathcal{E}}_{gen}$  using the Free Energy as a Generating Function, and how these errors are related to each other in the AA and High-T limit.

**4.2.6 The Thermodynamic limit.** In Section 4.2.7, we discuss the Large- $\mathcal{N}$  Thermodynamic limit and the Saddle Point Approximation (SPA), along with the concepts of Self-Averaging and Wick rotations.

**4.2.7 From the ST Perceptron to a Matrix Model.** Finally, in Section 4.2.8, we introduce the physical concepts necessary to understand the SETOL matrix model, including the Wide Layer Large- $\mathcal{N}$  limit and the notion of Size-Consistency. We then describe how to obtain the Layer Quality  $\bar{\mathcal{Q}}$  from a matrix-generalized Thermal Average over random matrices, called an HCIZ integral.

The various symbols and other important results are summarized in the Appendix A.1

## 4.2.1 Setup

In formulating SETOL, we want a methodology to estimate quantities such as the generalization error and/or accuracy that does not rely on traditional methods that split the data into training



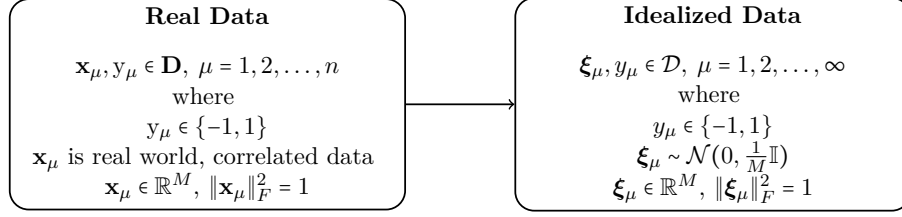


Figure 7: Mapping from a fixed set of  $n$  real-world, correlated data instances  $[\mathbf{x}, y] \in \mathbf{D}$  to an uncorrelated, random model of idealized data  $[\boldsymbol{\xi}, y] \in \mathcal{D}$ , drawn from a Gaussian i.i.d. distribution.

and test sets because **SETOL** makes *data independent* predictions. To accomplish this, we idealize the empirical data distribution as Gaussian fields, and we will use **StatMech** to construct quantities (basically, free energies or generating functions) so that we can compute training/testing errors by taking appropriate derivatives of these quantities.

In more detail, we imagine training a NN on  $n$  training data instances,  $\mathbf{x}_\mu$ , which are  $m$ -dimensional vectors, with labels  $y_\mu$ , chosen from a large but finite-size training data set  $\mathbf{D}$ . The goal of training a perceptron (or, later, a NN) is to learn the  $m$  weights of the vector  $\mathbf{w}$  (or, later, a weight matrix  $\mathbf{W}$ ) by running a form of stochastic gradient descent (SGD) to minimizing a loss function  $\mathcal{L}$  ( $\ell_2$ , cross-entropy, etc.). We want to approximate the actual network’s learning dynamics by an analytically tractable ensemble so that we can then obtain analytic expressions for the *Free Energy* and *Generating Function* we then use to compute Thermodynamic averages such as the *Average Generalization Error* ( $\mathcal{E}_{gen}$ ) and *Model Quality* ( $\mathcal{Q}$ ) (which is our approximation to the *Average Generalization Accuracy*).

**Counting Samples and Features.** We let the number of training samples be  $n$  and the dimension (i.e., number of features) for each sample be  $m$ . When we move to **SETOL** matrix-model, there will still be  $n$  training examples, but treated implicitly. The  $m$ -dimensional weight vector  $\mathbf{w}$  will become an  $N \times M$  weight matrix,  $\mathbf{W}$ , ( $N \geq M$ ) described as having  $N$  number of  $M$ -dimensional (input) feature vectors. Table 4 summarizes these conventions.

Definition	Vector	Matrix
Total number of data samples used in training.	$n$	$n$
Number of features per training sample (Input dimension).	$m$	$M$
Dimension of layer output (Output dimension)	1	$N$
Number of free parameters (in $R$ )	1	$M(M-1)/2$
Energy scaling	$n$	$n \times N \times M$

Table 4: In the ST Perceptron *vector* model, lowercase  $m$  is the dimension of the weight vector (total parameters), which is also the number of features per sample. In the vector case, there is one free parameter – the overlap  $R$  (or angle  $\theta$ ) between student and teacher. In the **SETOL** *matrix* model, uppercase  $N$  and  $M$  are the input and output dimensions of the weight matrix, and the matrix the overlap  $\mathbf{R}$ , being an  $M \times M$  symmetric matrix, has  $M(M-1)/2$  free parameters. The Energy scales as  $n$  in the ST Perceptron model, and as  $n \times N \times M$  in the **SETOL** matrix model.

**Actual and Idealized Data and Energies.** Consider a large set  $n$  of actual, real-world data,

$$(\mathbf{x}_\mu, y_\mu) \in \mathbf{D}, \mu = 1, \dots, n, \quad (17)$$

where  $\mathbf{x}_\mu \in \mathbb{R}^m$  is an  $m$ -dimensional real vector,  $y_\mu$  is a binary label taking values  $\{-1, 1\}$ , and  $\mathbf{D}$  denotes the finite-size dataset. WLOG, we assume that  $\mathbf{x}_\mu$  is normalized such that the norm squared is unity:

$$\|\mathbf{x}_\mu\|^2 := \sum_{i=1}^m \mathbf{x}_{\mu,i}^2 = 1 \quad (18)$$

We call  $\mathbf{x}^n$  an  $n$ -sized sample (of the training data instances  $\mathbf{x}$ ) from  $\mathbf{D}$ .

We define model errors as an energy  $E_{\mathcal{L}}$ , the difference squared between the Student's and Teacher's output. Smaller energies correspond to smaller errors and therefore better models. For example, for the mean-squared-error (MSE) loss, one has

$$E_{\mathcal{L}}(\mathbf{w}, \mathbf{x}_\mu, y_\mu) := (y_\mu - E_{NN}^{out}(\mathbf{w}, \mathbf{x}_\mu))^2, \quad (19)$$

where  $E_{NN}^{out}(\mathbf{w}, \mathbf{x}_\mu)$  is output prediction of the NN, as in Eqn. 1.<sup>19</sup>

We assume that there is a real-world training process that generates a Teacher model ( $T$ ), trained on a particular dataset  $\mathbf{D}$ , and we seek a theory for the Quality (or generalization accuracy) of this model. To estimate quantities such as the generalization error or generalization accuracy, we will adopt an approach that starts off by assuming idealized Gaussian data  $\mathcal{D}$ , but ends with the NN with a parametric model that we will fit with a Semi-Empirical procedure (described later). To that end, in the theoretical setup, the replacement scheme is,

$$\mathbf{D} \rightarrow \mathcal{D}, \quad \mathbf{x}_\mu \rightarrow \boldsymbol{\xi}_\mu, \quad y_\mu \rightarrow y_\mu, \quad (20)$$

where we denote the model training and/or test data instances as  $(\boldsymbol{\xi}, y)$  such that

$$(\boldsymbol{\xi}_\mu, y_\mu) \sim \mathcal{D}, \quad \mu = 1, \dots, \infty. \quad (21)$$

Here,  $\boldsymbol{\xi}_\mu \in \mathbb{R}^m$  is a random vector (i.e., an  $m$ -dimensional random variable), sampled from an i.i.d  $m$ -dimensional joint distribution  $\mathcal{D}$  of both the features  $\boldsymbol{\xi}_\mu$ , which are Gaussian, and the labels  $y_\mu$ , which are binary NN outputs.

#### 4.2.2 BraKets, Expected Values, and Thermal Averages

Given the setup from Section 4.2.1, we will treat the total energy  $E_{\mathcal{L}}^n(\mathbf{w}, \mathbf{x}^n)$  as a sum over some  $n$ -size data set  $\mathbf{x}^n$ . We can write the Total Data Sample Error, using an overloaded operator notation, as

$$E_{\mathcal{L}}^n(\mathbf{w}, \mathbf{x}^n, y^n) := \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \mathbf{x}_\mu, y_\mu), \quad (22)$$

where the superscript  $n$  in  $E_{\mathcal{L}}^n(\mathbf{w}, \mathbf{x}^n, y^n)$  indicates this is a sum over the entire set of  $n$  pairs  $[\mathbf{x}^n, y^n]$ . We should keep in mind that this depends on the specific set of  $n$  data pairs  $[(\mathbf{x}_\mu, y_\mu) \in \mathbf{D} \mid \mu = 1, \dots, n]$ . Here, we treat the labels  $y$  as *implicit* in  $E_{\mathcal{L}}^n(\mathbf{w}, \mathbf{x}^n)$ . We will therefore drop the  $y_\mu$  and  $y^n$  symbols, and simply write this total error / energy difference as

$$E_{\mathcal{L}}^n(\mathbf{w}, \mathbf{x}^n) := \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \mathbf{x}_\mu), \quad (23)$$

<sup>19</sup>Note that the Energy Landscape function  $E_{NN}^{out}$  is nonlinearly related to  $E_{\mathcal{L}}$ . We treat  $E_{NN}^{out}$  and  $E_{\mathcal{L}}$  as being the energy states of two separate, but interacting, thermodynamic systems, and the loss function  $\mathcal{L}$  is a transfer function that relates them.

1121 which is now a function of the entire set of  $n$  vectors  $[\mathbf{x}^n]$ .<sup>20</sup> This operator notation will prove  
 1122 useful later in Section 4.3.2 (see Eqn. 86) and in Appendix A.2.

1123 We will not, however, work directly with samples and sample averages. Instead, we will model  
 1124 them. To that end, we need to estimate them with a theoretical approach. For example, we can  
 1125 write the Total Data Sample Error in terms of our random data variables  $\xi^n$ , written formally as

$$E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) := \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \xi_{\mu}), \quad (24)$$

1126 but to evaluate this we need to take an integral and/or Expected Value over the data sample  $\xi^n$ .

1127 **Expected Values.** We need to compute various sums and integrals, sampling from a *idealized*  
 1128  $\mathcal{D}$  for the *actual* (i.e, real-world) data distribution  $\mathbf{D}$ , over  $n$ -sized data samples (or data sets), and  
 1129 also over distributions of weights  $(\mathbf{w}, \mathbf{s})$  and weight matrices  $(\mathbf{W}, \mathbf{S}, \mathbf{A}, \dots)$ . This will frequently  
 1130 (but not always) be defined as more familiar Expected Values. We will denote Expected Values  
 1131 using physics Bra-Ket notation. Importantly, we use the term Expected Value in the physics  
 1132 sense, and BraKets will denote an un-normalized sum or integral; when the quantity is to be  
 1133 normalized, we will denote the normalization explicitly. For example, given a function  $f(\xi)$ , we  
 1134 write the BraKet integral as:

$$\langle f(\xi) \rangle_{\xi} := \int d\mu(\xi) f(\xi). \quad (25)$$

1135 We would express an  $n$ -sized sample average over  $f()$  as

$$\begin{aligned} \langle f(\xi^n) \rangle_{\xi^n} &:= \frac{1}{n} \int d\mu(\xi^n) f(\xi^n) \\ &= \frac{1}{n} \left[ \prod_{\mu=1}^n \int d\xi_{\mu} P(\xi_{\mu}) \right] \left[ \sum_{\mu=1}^n f(\xi_{\mu}) \right]. \end{aligned} \quad (26)$$

1136 The BraKet  $\langle \dots \rangle_{\xi^n}$  denotes an integral over an  $n$ -sized sample of idealized Gaussian-field data  
 1137  $\xi^n$ , with the convention that summation over  $n$  points and normalization  $\frac{1}{n}$  appears inside the  
 1138 Bra-Ket implicitly.

1139 For example, we treat an Expected Value of the Data Sample Error, which is correlated  
 1140 when using real-world data  $\mathbf{D}$ , using the uncorrelated idealized data  $\mathcal{D}$ ; this is specified with the  
 1141 following mapping:

$$\frac{1}{n} E_{\mathcal{L}}^n(\mathbf{w}, \mathbf{x}^n) \xrightarrow{\text{Expected Value}} \langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\xi^n}, \quad (27)$$

1142 where the BraKet  $\langle \dots \rangle_{\xi^n}$  denotes the integral over the idealized dataset  $\xi^n$  of a normalized average  
 1143 over the sample. In this case, we obtain:

$$\begin{aligned} \langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\xi^n} &:= \frac{1}{n} \int d\mu(\xi^n) E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \\ &= \frac{1}{n} \int \left[ \prod_{\mu=1}^n d\xi_{\mu} P(\xi_{\mu}) \right] \left[ \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \xi_{\mu}) \right], \\ &= \frac{1}{n} \sum_{\mu=1}^n \int d\xi_{\mu} P(\xi_{\mu}) E_{\mathcal{L}}(\mathbf{w}, \xi_{\mu}), \end{aligned} \quad (28)$$

<sup>20</sup>In the classic Student Teacher model, the labels  $y^n$  represent the Teacher outputs and are effectively treated as either uniform random variables to be averaged over later, or as the outputs of an optimal Teacher. In this work, the Teacher weights  $\mathbf{w}$ , not labels, are input (i.e., a fixed ESD, later) so we can drop the labels.

where  $P(\xi^n)$  is a product of  $n$  i.i.d.  $m$ -dimensional Gaussian distributions. The subscript  $\bar{\xi^n}$  indicates this is an Expected Value of an average of an  $n$ -size *sample* of ideal data, where the Expected Value is taken over datasets, and the average is over data points within each sample. The third line follows because the  $n$  samples are i.i.d. (This is used in both Sections 4 and 5.) (The normalization  $\frac{1}{n}$  ensures the Bra-Ket is a proper Expected Value of a sample average.) The measure  $d\mu(\xi^n)$  denotes the probability measure associated with a single *realization* of a random data sample of size  $n$  drawn from an  $m$ -dimensional idealized Gaussian distribution. A subscript  $\xi$  on the Ket as  $\langle \dots \rangle_\xi$  indicates that the integral is over potential data points, not an average of a data sample (i.e., there would be no  $1/n$  prefactor).

**Size-Extensivity and Size-Intensivity.** A key requirement for the Thermodynamic limit in StatMech is *Size-Extensivity*: that physically meaningful quantities (i.e, total energies and free energies) scale linearly with the system size or number of parameters, i.e.  $m$  (or  $N \times M$ , below). Extensive quantities scale with system size, intensive ones do not. Along with this, Thermodynamic average quantities should be *Size-Intensive*, meaning that they remain independent of  $n$  (or  $N \times M$ , below) as the system size increases. In our setting, Size-Extensivity and Size-Intensivity underpin the so-called Large- $\mathcal{N}$  limits we employ, ensuring that macroscopic observables become independent of microscopic fluctuations so that the system approaches equilibrium as expected.

In the theory of the Statistical Mechanics of Generalization (SMOG), however, one also holds the (feature) load  $= n/m$  fixed when taking the Thermodynamic limit, and we will do the same [90, 8, 91, 93]. In fact, we will take load to be unity, and not treat it explicitly.<sup>21</sup> Moreover, we will use  $n$  as the primary variable below as we are interested in how the Free Energy and other quantities change with  $n$ . That is, we use the notational convention in [10] (as opposed to [8]). **Consequently, for our purposes here, this means that the Thermodynamic limit and the ‘Large- $\mathcal{N}$  limit in  $n$ ’ are effectively the same.**

As an example of Size-Extensivity and Size-Intensivity, we write the Expected Value (i.e., the data-average) of Data Sample Error  $E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)$  (Eqn. 28) in the Large- $\mathcal{N}$  limit in  $n$  as

$$\lim_{n \gg 1} \langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\bar{\xi^n}} = \lim_{n \gg 1} \frac{1}{n} \int \left[ \prod_{\mu=1}^n d\xi_\mu P(\xi^n) \right] \left[ \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \xi_\mu) \right]. \quad (29)$$

Here, the notation ( $n \gg 1$ ) means  $n$  grows arbitrarily large, but is not necessarily at the limit point ( $n = \infty$ ). And, again, the load is fixed, so  $n \gg 1 \leftrightarrow m \gg 1$ . The Total Data Sample Error  $E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)$  is Size-Extensive, whereas the average  $\langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\bar{\xi^n}}$  is Size-Intensive. This limit will be implicit later when taking a Saddle Point Approximation (see below).<sup>22</sup>

The data-averaged error  $\langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\bar{\xi^n}}$  will appear frequently below. For convenience and for compatibility with [8], we denote it using the symbol  $\epsilon(\mathbf{w})$ :

$$\epsilon(\mathbf{w}) := \lim_{n \gg 1} \langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\bar{\xi^n}} \quad (\text{Size-Intensive}). \quad (30)$$

where, by our normalization here,  $\epsilon(\mathbf{w}) \in [0, 1]$ . The symbol  $\epsilon(\mathbf{w})$  is our theoretical estimate of the sample average  $E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)$  (Eqn. 29), well-defined for any  $n$ . We also call  $\epsilon(\mathbf{w})$  the *Annealed Error Potential*, which will be made clear below.

<sup>21</sup>For our purposes, we only require that  $n/m$  is *some fixed quantity* as we take this limit. We note that  $n/m = 1$  is the Double Descent Worst Case, however assuming that  $n/m$  is some other constant addresses this without changing any of the results.

<sup>22</sup>As we are working within a “physics-level of rigor”, we take some liberties in evaluating these Large- $\mathcal{N}$  limits; and we leave the formal proofs for future work.

1179 It is also convenient to write *Total Annealed Error Potential* as an Energy,

$$\mathcal{E}(\mathbf{w}) := n\epsilon(\mathbf{w}) \quad (\text{Size-Extensive}). \quad (31)$$

1180 This will only be useful when the Thermodynamic limit exists, and this can be reasonably expected  
1181 for the Annealed Approximation (AA), which is the regime in which SETOL will be developed.<sup>23</sup>

1182 **From Errors to Accuracies: The Average Generalization Accuracy, the Quality, and**  
1183 **the Self-Overlap.** We have been discussing various forms of errors. In SETOL, we will, how-  
1184 ever, primarily be concerned with approximating the *Average Generalization Accuracy*, or, more  
1185 generally, the Quality of a NN model and/or its layers.<sup>24</sup> The average accuracy is simply one  
1186 minus the error. To represent this, we introduce the *Self-Overlap*  $\eta(\mathbf{w})$ , which is defined generally  
1187 as

$$\eta(\mathbf{w}) := 1 - \epsilon(\mathbf{w}), \quad \eta(\mathbf{w}) \in [0, 1], \quad (32)$$

1188 and which describes the “overlap” between the true and the predicted labels. Unlike here, however,  
1189 in later sections (4.3.2, 5.1, and Appendix A.3) we will first define a data-dependent Self-Overlap,  
1190 so that we may obtain  $\eta(\mathbf{w}) := \langle \eta(\mathbf{w}, \xi) \rangle_{\xi^n}$  directly.

1191 **Bracket Notation.** We will use physics Bra-Ket notation,  $\langle \dots \rangle$ , to denote different kinds of sums  
1192 and integrals, with superscripts and subscripts, and for Expected Values (estimated theoretical  
1193 averages). We use superscripts to denote the kind of integral or average:

1194 Thermal  $\langle \dots \rangle^\beta$ , Annealed  $\langle \dots \rangle^{an}$ , high-T  $\langle \dots \rangle^{hT}$ , HCIZ  $\langle \dots \rangle^{IZ}$ , etc.

1195 We use subscripts to emphasize the dependent variables:

1196 weights  $\langle \dots \rangle_{\mathbf{w}}$ ,  $\langle \dots \rangle_{\mathbf{s}}$ ,  $\langle \dots \rangle_{\mathbf{s}}$

1197 data  $\langle \dots \rangle_{\xi}$ ,  $\langle \dots \rangle_{\xi^n}$ ,  $\langle \dots \rangle_{\xi^n}$

1198 When averaging over whole datasets  $\xi^n$ , the subscript will appear with a bar (i.e.  $\xi^n$ ), but when  
1199 just integrating over a particular dataset, no bar will appear (i.e.,  $\xi^n$ ). We also reuse these  
1200 symbols for other quantities, such as the  $Z_n^{an, hT}$ ,  $\bar{\mathcal{E}}_{gen}^{an, hT}$ ,  $H^{an}(\mathbf{w})$ , etc, but may mix-and-match  
1201 subscripts and superscripts for visual clarity.

1202 **Sign Conventions.** Finally, we discuss the sign conventions used. Since errors decrease with  
1203 better models, Energies ( $E_{\mathcal{L}}(\mathbf{w}, \xi)$ ,  $\mathcal{E}(\mathbf{w})$ ,  $\epsilon(\mathbf{w})$ , ...) and Free Energies ( $F$ ) are minimized to obtain  
1204 better models. Likewise, since accuracies increase with better models, Qualities ( $\bar{Q}$ ,  $\bar{Q}^2$ , ...), Self-  
1205 Overlap ( $\eta$ ), and Quality Generating Function ( $\Gamma$ ) would be maximized to obtain better models.  
1206 An exception will be Hamiltonians ( $H$ ,  $\mathbf{H}$ ), where the sign convention will depend on context.

<sup>23</sup>We should note that, while our model training and generalization errors are always expressed as energies, an energy is not necessarily a model error.

<sup>24</sup>Technically, the Quality will estimate the average *Precision* rather than the Accuracy. This will distinction will be clarified in the Section 4.3.

1207 **Thermal Averages (over weights).** To evaluate the expectation value of some equilibrium  
 1208 quantity that depends on the weights  $\mathbf{w}$  (say  $\mathbb{E}_{\mathbf{w}}^{\beta}[f(\mathbf{w})]$ ), one uses a Thermal Average. By this,  
 1209 we mean a *Boltzmann-weighted average*: given a function  $f(\mathbf{w})$ , we define the Thermal Average  
 1210 over  $\mathbf{w}$  as

$$\langle f(\mathbf{w}) \rangle_{\mathbf{w}}^{\beta} := \frac{1}{Z_n} \int d\mu(\mathbf{w}) f(\mathbf{w}) e^{-\beta \mathcal{E}(\mathbf{w})}, \quad (33)$$

1211 where the superscript  $\beta$  denotes Thermal Average,  $\beta = \frac{1}{T}$  is an inverse temperature, and  $Z_n$  is  
 1212 the normalization term (or Partition function), defined as

$$Z_n := \int d\mu(\mathbf{w}) e^{-\beta \mathcal{E}(\mathbf{w})}, \quad (34)$$

1213 defined for the  $n$ -size *Data Sample*  $\xi^n$ . In particular, when we want to compute the Thermal  
 1214 Average of the *Total Energy* difference or Error  $\mathcal{E}(\mathbf{w})$  over  $\mathbf{w}$ , we could write

$$\langle \mathcal{E}(\mathbf{w}) \rangle_{\mathbf{w}}^{\beta} := \frac{1}{Z_n} \int d\mu(\mathbf{w}) \mathcal{E}(\mathbf{w}) e^{-\beta \mathcal{E}(\mathbf{w})}. \quad (35)$$

1215 Importantly, we will never calculate the average errors directly like this. Instead, we will calculate  
 1216 them from partial derivatives of the Free Energy  $F_n$  (as shown below). Also, we may use  $\langle \dots \rangle_{\xi^n}^{\beta}$   
 1217 to denote what looks like a Thermal Average over the data; this is not essential and only used  
 1218 once below and can be ignored for this section.

1219 **Other Notation: Overbars, Superscripts and Subscripts.** As above, we may also occa-  
 1220 sionally denote averages using the common notation for expected values,  $\mathbb{E}[\dots]$ . See Table 11  
 1221 and 12 in Appendix A for a list of these and other notational conventions and symbols we use.

1222 When discussing quantities such as the Free Energy ( $F$ ), training and test errors/eneries ( $\mathcal{E}$ ),  
 1223 the Layer Quality ( $\mathcal{Q}$ ), etc., we will place a bar over the symbol (i.e.,  $\bar{F}$ ,  $\bar{\mathcal{E}}$ ,  $\bar{\mathcal{Q}}$ , etc.) when referring  
 1224 to an average over the data  $n$ . Otherwise, we will refer to these quantities as the total (averaged)  
 1225 energy, error, quality, etc.

1226 Finally, when referring to the model (i.e., theoretical) training and generalization errors, we  
 1227 will use the superscript  $ST$  for the average Student-Teacher training and generalization errors,  
 1228  $\bar{\mathcal{E}}_{train}^{ST}$  and  $\bar{\mathcal{E}}_{gen}^{ST}$ , respectively, and the superscript  $NN$  for the matrix-generalized NN layer average  
 1229 training and generalization errors,  $\bar{\mathcal{E}}_{train}^{NN}$  and  $\bar{\mathcal{E}}_{gen}^{NN}$ , respectively. When referring to empirical  
 1230 errors, we denoted these as  $\bar{\mathcal{E}}_{train}^{emp}$  and  $\bar{\mathcal{E}}_{gen}^{emp}$ , respectively.

### 1231 4.2.3 Free Energies and Generating Functions

1232 If one needs an average energy (or error), it is often easier to calculate the associated Free Energy  
 1233 and take corresponding partial derivatives than it is to compute that quantity directly via an  
 1234 expected value or Thermal Average. Generally speaking, a Free Energy,  $F_n$ , is defined in terms  
 1235 of a partition function  $Z_n$  as

$$\beta F_n := -\ln Z_n. \quad (36)$$

1236 Keep in mind that  $Z_n$  may actually be a function of the idealized data  $\xi$  (or some other variables),  
 1237 i.e.,  $Z(\xi)$ , but we usually don't write this explicitly. Likewise, while both  $F_n$  and  $Z_n$  depend  
 1238 explicitly on the system size  $n$ , we will only include these subscripts when emphasizing this. Also,  
 1239  $F_n$  has units of Energy or Temperature, so  $\beta F_n = -\ln Z_n$  is a "unitless" Free Energy. Each model  
 1240 (in single-layer models) and/or layer (in multi-layer models) will have its own Partition Function



and associated Generating Functions. We call  $F_n$  and  $Z_n$  *Generating Functions* because they can be used to generate the model errors. That is, given an  $F_n$  and/or  $Z_n$ , we can “generate” the training and generalization errors with the appropriate partial derivatives w.r.t  $\beta$  and  $n$  [9, 10].

From this generating function perspective, i.e., when using a generating function to compute quantities of interest, we can work with other transformations of  $F_n$ . Most notably, we will consider

$$\Gamma_n = n - F_n. \quad (37)$$

where we note that these Energies scale as  $n$  for the ST vector model, but for a matrix model they scale as  $n \times N \times M$ ; see Appendix A.2.1). The quantity  $\Gamma_n$  decreases as the error increases (as opposed to  $F_n$ , which increases), i.e., it increases as the accuracy of quality of the model increases. Thus, we will use it as a generating function for the model quality/accuracy. For average Qualities, one has

$$\bar{\Gamma}_n := 1 - \bar{F}_n \quad (38)$$

for the model or layer under consideration (see below).

#### 4.2.4 The Annealed Approximation (AA) and the High-Temperature Approximation (high-T)

In the traditional SMOG approach, one models the (typical) generalization behavior of a NN by defining and computing the Expected Value of the Free Energy of the model. The full expected value of the Free Energy,  $\beta F_n = -\ln Z_n$ , with respect to the (idealized) data  $\xi^n$ , is:

$$\mathbb{E}_{\xi^n}[\beta F_n] = \beta \bar{F}_n := -\langle \ln Z_n \rangle_{\xi^n}, \quad (39)$$

where  $\langle \ln Z_n \rangle_{\xi^n}$  means where we average over the  $n$  samples of the data ( $\xi^n$ , of size  $n$ ). This is also called the Quenched Free Energy. This is, however, frequently too difficult to analyze, and doing so typically requires a so-called Replica calculation.

The Annealed Approximation (AA) is a way of taking the data-average *first* and greatly simplifies the model under study and its analysis. The standard way to move forward is to follow the methods used in disordered systems theory [8, 5]. The mapping is:

Average over the Data	$\leftrightarrow$	Annealed Approximation	$\leftrightarrow$	Disorder Average
Learning the Weights	$\leftrightarrow$	NN Optimization Algorithm	$\leftrightarrow$	Thermal Average.

through the NN optimization algorithm, and then evaluates the training or test accuracy by averaging over the (actual) data  $\mathbf{x}^n$ . In the theoretical analysis, however, the steps are reversed. One first averages over the (model) data  $\xi^n$  (i.e., a multi-variate Gaussian distribution) so that the disorder (variability in the data) is averaged out. Then, a Thermal Average is used to model the final state of NN learning process, the learned weights.

**The Annealed Approximation (AA).** Formally, the AA makes the substitution

$$-\langle \ln Z_n \rangle_{\xi^n} \approx -\ln \langle Z_n \rangle_{\xi^n}. \quad (40)$$

Here, we are *averaging over the disorder*. We may associate:

$$\begin{aligned} -\beta \langle \ln Z_n(\xi^n) \rangle_{\xi^n} &: \text{the Quenched Free Energy} \\ -\beta \ln \langle Z_n(\xi^n) \rangle_{\xi^n} &: \text{the Annealed Free Energy.} \end{aligned}$$

1271 Applying the AA amounts to applying Jensens inequality *as an equality*, and it allows will let us  
 1272 interchange integrals and logarithms when computing the data average:

$$\frac{1}{n} \int d\mu(\xi^n) \ln(\dots) \xrightarrow{\text{AA}} \ln \frac{1}{n} \int d\mu(\xi^n)(\dots) \quad (41)$$

1273 This will allow us to switch the order of the data and the thermal averages, i.e.,

$$\left\langle \langle \dots \rangle_{\mathbf{w}}^\beta \right\rangle_{\xi^n} \xrightarrow{\text{AA}} \left\langle \langle \dots \rangle_{\xi^n}^\beta \right\rangle_{\mathbf{w}}, \quad (42)$$

1274 greatly simplifying the analysis.

1275 The use of the AA is common in **StatMech**, as it simplifies computations considerably; and it  
 1276 is chosen when it holds exactly (if, say,  $x$  is a typical sample from  $\mathcal{D}$  and  $Z_w(\xi)$  has a well-defined  
 1277 mean). In contrast, there are situations in **StatMech** when the average is atypical, and then it  
 1278 one can get different results for the Quenched versus Annealed cases. In a practical sense, one  
 1279 imagines this may occur when the data is very noisy and/or mislabeled, and this requires a special  
 1280 treatment [8].

1281 **Annealed Hamiltonian  $H^{an}(\mathbf{w})$  and Annealed Partition Function  $Z^{an}$ .** When we apply  
 1282 the AA (as in Eqn. 41), we average over the data  $\xi^n$  first. Doing this will allow us to develop a  
 1283 theory in terms a (Temperature dependent) Annealed Error Potential.

1284 Following [8] (see their Eqn.(2.30)), we will call this average the *Annealed Hamiltonian*,  
 1285  $H^{an}(\mathbf{w})$ , which we define as

$$\beta H^{an}(\mathbf{w}) := -\frac{1}{n} \ln \int d\mu(\xi^n) e^{-\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)}. \quad (43)$$

1286 The Annealed Hamiltonian is a simple “mean-field-like” Hamiltonian for the problem. This can  
 1287 be seen by noting that we can express Eqn. 43 as an integral over a single data example  $\xi$ :

$$\begin{aligned} \beta H^{an}(\mathbf{w}) &= -\frac{1}{n} \ln \int d\mu(\xi^n) e^{-\beta \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \xi_\mu)} \\ &= -\ln \left[ \int d\mu(\xi^n) e^{-\beta \sum_{\mu=1}^n E_{\mathcal{L}}(\mathbf{w}, \xi_\mu)} \right]^{\frac{1}{n}} \\ &= -\ln \left[ \prod_{\mu=1}^n \int d\mu(\xi_\mu) e^{-\beta E_{\mathcal{L}}(\mathbf{w}, \xi_\mu)} \right]^{\frac{1}{n}} \\ &= -\ln \int d\mu(\xi) e^{-\beta E_{\mathcal{L}}(\mathbf{w}, \xi)} \end{aligned} \quad (44)$$

$$= -\ln \int d\mu(\xi) e^{-\beta E_{\mathcal{L}}(\mathbf{w}, \xi)} \quad (45)$$

1288 This will be a critical piece needed to generalize the vector-based ST Perceptron model to the  
 1289 matrix-generalized ST MLP model. In BraKet notation, Eqn. 45 can be expressed as

$$\beta H^{an}(\mathbf{w}) := -\frac{1}{n} \ln \left\langle e^{-\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)} \right\rangle_{\xi^n} = -\ln \left\langle e^{-\beta E_{\mathcal{L}}(\mathbf{w}, \xi)} \right\rangle_{\xi}.$$

1290 Using  $H^{an}(\mathbf{w})$ , we can define the *Annealed Partition Function*,  $Z_n^{an}$ , as

$$\begin{aligned} Z_n^{an} &:= \int d\mu(\mathbf{w}) e^{-n\beta H^{an}(\mathbf{w})} \\ &= \int d\mu(\mathbf{w}) \exp \left[ -n \left( -\frac{1}{n} \ln \int d\mu(\xi^n) e^{-\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)} \right) \right] \\ &= \int d\mu(\mathbf{w}) \exp \left[ \ln \int d\mu(\xi^n) e^{-\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)} \right] \\ &= \int d\mu(\mathbf{w}) \int d\mu(\xi^n) e^{-\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)}. \end{aligned} \quad (46)$$

$$= \int d\mu(\mathbf{w}) \int d\mu(\xi^n) e^{-\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)}. \quad (47)$$

where the lines after the first line follow by substituting Eqn. 43 into Eqn. 46. Note also that the order of the integrals in Eqn. 47 is exactly what we expect using the AA, as in Eqn. 42. Also, analogously to Eqn. 45, we can write  $Z_n^{an}$  as the product of the  $n = 1$  case,  $Z_n^{an} = [Z_1^{an}]^n$ . Finally, we will only need the high-T version,  $H_{hT}^{an}$ , of  $H^{an}(\mathbf{w})$ , and this will take a very simple form. <sup>25</sup>

**The High-Temperature (High-T) Annealed Hamiltonian ( $H_{hT}^{an}(\mathbf{w}) = \epsilon(\mathbf{w})$ ) and Partition Function ( $Z_n^{an, hT}$ ).** In addition to the AA, we will be evaluating our models at high-T. Notably, the Annealed Hamiltonian  $H^{an}(\mathbf{w})$  in Eqn. 43 is a non-linear function of  $\beta$ ; by taking the high-T approximation, we can remove this dependence and obtain the simpler expression that  $H^{an}(\mathbf{w}) = \epsilon(\mathbf{w})$ . This greatly simplifies both the Partition Function, i.e.,  $Z_n^{an, hT}$ , and subsequent results (below).

To obtain the high-T result, we can write the Taylor expansion for  $e^{\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)}$  and keep the first two terms:

$$e^{-n\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)} \simeq 1 - \underbrace{\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)}_{\text{high-T}} + (\beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n))^2 + \dots \quad (48)$$

Let us now express  $H^{an}(\mathbf{w})$  directly in terms of  $\epsilon(\mathbf{w}) = \langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\xi^n}^-$  (see Eqn. 30) as a Thermal Average at high-T. To do so, let's take a high-T expansion of Eqn. 43 by expanding the exponential to first order in  $\beta$ , to obtain

$$\begin{aligned} \beta H_{hT}^{an}(\mathbf{w}) &= -\frac{1}{n} \ln \int d\mu(\xi^n) [1 - \beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)] \\ &\approx -\frac{1}{n} \int d\mu(\xi^n) \beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \\ &= \langle \beta E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\xi^n}^- \\ &= \frac{1}{n} \beta (\mathcal{E}(\mathbf{w})) \\ &= \beta \epsilon(\mathbf{w}). \end{aligned} \quad (49)$$

Here, we have used the AA, and the property that  $\ln(1 + y) \approx y$ , for  $|y| \ll 1$ , and the fact that  $\epsilon(\mathbf{w})$  takes the form given in Eqn. 30. This gives  $H_{hT}^{an}(\mathbf{w}) := \epsilon(\mathbf{w})$ , which is no longer a non-linear function of  $\beta$ . Moving forward, we will assume we are taking the high-T limit like this.

Given Eqn. 49, we can now express the Annealed Partition Function at high-T directly in terms of the Annealed (i.e., data-averaged) error  $\epsilon(\mathbf{w})$ :

$$\begin{aligned} Z_n^{an, hT} &:= \int d\mu(\mathbf{w}) e^{-n\beta H_{hT}^{an}(\mathbf{w})} \\ &= \int d\mu(\mathbf{w}) e^{-n\beta \epsilon(\mathbf{w})} \end{aligned} \quad (50)$$

If we assume that at high-T we can make this approximation, since we only care about the small  $\beta$  results. This will prove very useful later when working with HCIZ integrals.

#### 4.2.5 Average Training and Generalization Errors and their Generating Functions

Here, we show how to derive the Average Training Error  $\bar{\mathcal{E}}_{train}$  and the Average Generalization Error  $\bar{\mathcal{E}}_{gen}$ , in the Annealed Approximation (AA), and at high-Temperature (high-T), using the

<sup>25</sup>We will derive expressions for  $\epsilon(R)$  and  $\bar{\mathcal{E}}_{gen}^{ST}(R)$  in Eqn. 97 and Eqn. 98, respectively, using relatively simple arguments. In Appendix A.2.1 we present a more detailed derivation of  $H^{an}(R)$  and  $H_{hT}^{an}(R) = \epsilon(R)$  in Appendix A.2.2 we show that these derivations generalize to the matrix-generalized case,  $H^{an}(\mathbf{R})$ .

Free Energy  $F_n$  and/or the Partition Function  $Z_n$  as a generating function. In particular, we show that, in the AA and at high-T, these errors are (approximately) equal and equal to the Thermal Average of the Annealed Error Potential,  $\bar{\mathcal{E}}_{train}^{an,hT} \approx \bar{\mathcal{E}}_{gen}^{an,hT} \approx \langle \epsilon(\mathbf{w}) \rangle_{\mathbf{w}}^\beta$ .

**Generating Functions for the Errors: the StatMech way.** In our theory, after applying the AA, we obtain expressions where the random model data  $\xi^n$  has been integrated out. This leaves formal quantities that depend only on the weights  $\mathbf{w}$ , which are the variables being learned during training. Since we are left with a distribution over  $\mathbf{w}$ , we define the training error not explicitly as an average over the training data itself, but instead in terms of how the Free Energy,  $\beta F := -\ln Z_n$ , varies with  $\beta$ , i.e., the amount of stochasticity in the model weights.

Following [9, 10], we define the *Average Training Error*, in the AA, by differentiating  $\ln Z_n^{an}$  with respect to  $\beta$ :

$$\bar{\mathcal{E}}_{train}^{an} := -\frac{1}{n} \frac{\partial(\ln Z_n^{an})}{\partial \beta} = -\frac{1}{n} \frac{1}{Z_n} \frac{\partial Z_n^{an}}{\partial \beta}. \quad (51)$$

This error captures how the model predictions will vary with changes in the learned weights  $\mathbf{w}$ , which implicitly describes how the changes will vary with the training data  $\xi^n$ . Similarly, we define the *Average Generalization Error*, in the AA, by differentiating  $\ln Z_n^{an}$  with respect to  $n$ , the number of data points. Following

$$\bar{\mathcal{E}}_{gen}^{an} := -\frac{1}{\beta} \frac{\partial(\ln Z_n^{an})}{\partial n} + \frac{1}{\beta} \ln z(\beta) = -\frac{1}{\beta} \frac{1}{Z_n} \frac{\partial Z_n^{an}}{\partial n} + \frac{1}{\beta} \ln z(\beta), \quad (52)$$

where  $z(\beta)$  is a constant normalization term that depends only on  $\beta$  (which, moving forward, we ignore, as it only shifts the scale). This error captures how the model's predictions will change as more data points are introduced.

In the Thermodynamic limit ( $n \gg 1$ ), these two definitions of the error become equivalent at High-T, and they are equal to the Thermal Average of the Annealed Error Potential:

$$\bar{\mathcal{E}}_{train}^{an,hT} = \bar{\mathcal{E}}_{gen}^{an,hT} = \langle \epsilon(\mathbf{w}) \rangle_{\mathbf{w}}^\beta, n \gg 1. \quad (53)$$

To see this, substitute Eqn. 50 into Eqn. 51, and take the partial derivative w.r.t  $\beta$ , to obtain

$$\begin{aligned} \bar{\mathcal{E}}_{gen}^{an,hT} &:= \frac{1}{n} \frac{\partial(-\ln Z_n^{an,hT})}{\partial \beta} \\ &= -\frac{1}{n} \frac{\partial}{\partial \beta} \ln \int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})} \end{aligned} \quad (54)$$

$$\begin{aligned} &= \frac{\frac{1}{n} \int d\mu(\mathbf{w}) n\epsilon(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})}}{\int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})}} \\ &= \langle \epsilon(\mathbf{w}) \rangle_{\mathbf{w}}^\beta. \end{aligned} \quad (55)$$

Likewise, if we substitute Eqn. 50 into Eqn. 52, and take the partial derivative w.r.t.  $n$ , we obtain

$$\begin{aligned} \bar{\mathcal{E}}_{gen}^{an,hT} &:= \frac{1}{\beta} \frac{\partial(-\ln Z_n^{an,hT})}{\partial n} \\ &= -\frac{1}{n} \frac{\partial}{\partial \beta} \ln \int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})} \end{aligned} \quad (56)$$

$$\begin{aligned} &= \frac{\frac{1}{\beta} \int d\mu(\mathbf{w}) n\epsilon(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})}}{\int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})}} \\ &= \langle \epsilon(\mathbf{w}) \rangle_{\mathbf{w}}^\beta. \end{aligned} \quad (57)$$

1339 Notice that both of these results arise because of the simple expression that appears in the  
 1340 exponent of  $Z_n^{an,hT}$ , namely because  $-n\beta H_{hT}^{an}(\mathbf{w}) = n\beta\epsilon(\mathbf{w})$ .

1341 This equivalence reflects the fact that when the system is large enough, adding a new data  
 1342 example to the training distribution is formally equivalent to adding noise, making the two errors  
 1343 indistinguishable. This approach allows us to define both training and generalization errors in  
 1344 terms of fundamental thermodynamic quantities, providing a simplified formal framework suitable  
 1345 for empirical adjustment later.

1346 Also, note that the model data variables  $\xi$  do not enter the calculation because we integrated  
 1347 them out before the calculation of Thermal Average. (This illustrates the difference between  
 1348 taking an annealed versus a quenched average.) Also, our sign convention is consistent with a  
 1349 model of NN training that *minimizes* the total loss ( $\mathcal{L}$ ) and/or ST error, and, therefore minimizes  
 1350 Free Energies as well.

1351 More generally, we see that we can use the Partition Function,  $Z_n$ , and/or the Free Energy,  
 1352  $\beta F_n := -\ln Z_n$ , as a Generating Function to obtain any desired Thermodynamic average by taking  
 1353 the appropriate partial derivative of the corresponding form of  $\ln Z$ . In Appendix 4.2 we show  
 1354 how to obtain  $\bar{\mathcal{E}}_{train}^{an}$  and  $\bar{\mathcal{E}}_{gen}^{an}$  obtain explicitly in this way using  $Z^{an}$ .

#### 1355 4.2.6 The Quality ( $\bar{Q}$ ) and its Generating Function ( $\Gamma_{\bar{Q}}$ )

1356 Here, we explain how to define what we call the Quality  $\bar{Q}$ , which is defined as the Thermal  
 1357 Average of the Self-Overlap,  $\bar{Q} := \langle \eta(\mathbf{w}) \rangle_{\mathbf{w}}^\beta$ , and which can be obtained from the associated  
 1358 *Quality Generating Function*  $\Gamma_{\bar{Q}}$ . See Table 5 for a quick summary.

Symbol	Definition & Formula		Eq. #
$\epsilon$	Annealed Error Potential (Large- $\mathcal{N}$ , high-T)	$\epsilon(\mathbf{w}) = \langle E_{\mathcal{L}}^n(\mathbf{w}, \xi^n) \rangle_{\xi^n}$	30
$\eta$	Self-Overlap (average accuracy):	$\eta(\mathbf{w}) = 1 - \epsilon(\mathbf{w})$	32
$\bar{F}_n$	Average Free Energy:	$\beta \bar{F}_n = -\langle \ln Z_n \rangle_{\xi^n}$	39
$\Gamma_{\bar{Q}}$	Quality-Generating Function:	$\Gamma_{\bar{Q}} = 1 - \bar{F}_n$	38
$\bar{Q}$	Model Quality (average self-overlap):	$\bar{Q} = \langle \eta(\mathbf{w}) \rangle_{\mathbf{w}}^\beta$	60

Table 5: Summary of the main intensive (average, per-parameter) quantities. Here  $n$  is the number of free parameters. The average model Quality  $\bar{Q}$  is the model’s average accuracy (one minus the error), and the Quality-Generating function  $\Gamma_{\bar{Q}}$  plays the same role as the free energy  $\bar{F}$  but with an opposite sign convention.

1359 For our purposes below, we define the Model Quality (as in Eqn. 7) as our approximation to  
 1360 the Average Generalization Accuracy for our model. We denote the Model Quality for the ST  
 1361 Perceptron model,  $\bar{Q}^{ST}$ , and for a general NN,  $\bar{Q}^{NN}$ , such that

$$\bar{Q}^{ST} := 1 - \bar{\mathcal{E}}_{gen}^{ST} \quad (58)$$

$$\bar{Q}^{NN} := 1 - \bar{\mathcal{E}}_{gen}^{NN} \quad (59)$$

1362 In this work, however, the Quality will always be defined at high-T, and so we may write

$$\bar{Q}^{ST} = 1 - [\bar{\mathcal{E}}_{train}^{ST}]^{an,hT} = 1 - [\bar{\mathcal{E}}_{gen}^{ST}]^{an,hT} \quad (60)$$

$$\bar{Q}^{NN} = 1 - [\bar{\mathcal{E}}_{train}^{NN}]^{an,hT} = 1 - [\bar{\mathcal{E}}_{gen}^{NN}]^{an,hT} \quad (61)$$

1363 We also define a Layer Quality, simply denoted  $\bar{Q}$ , which will describe the contributions an  
 1364 individual layer makes to the overall Model Quality  $\bar{Q}^{NN}$ . To obtain the Layer Quality, we define  
 1365 an accuracy–or Quality–Generating Function, denoted  $\Gamma_{\bar{Q}}$ , which is analogous to a layer Free  
 1366 Energy, but with the opposite sign convention.

1367 Generally speaking, the Quality Generating Function  $\Gamma_{\bar{Q}}$  is defined in the AA, and at high-T  
 1368 and is given as

$$\beta\Gamma_{\bar{Q}} := \ln \int d\mu(\mathbf{w}) e^{n\beta\eta(\mathbf{w})} \quad (62)$$

1369 For example, for the single-layer ST Perceptron,  $\Gamma_{\bar{Q}ST} := n - F_n^{ST}$  (in units of energy or error).  
 1370 The term  $\Gamma_{\bar{Q}ST}$  is directly related to the *Total* Free Energy  $F_n^{ST}$ , which can be seen by substituting  
 1371 Eqn. 32 for  $\eta(\mathbf{w})$  in Eqn. 62:

$$\begin{aligned} \beta\Gamma_{\bar{Q}ST} &= \ln \int d\mu(\mathbf{w}) e^{n\beta(1-\epsilon(\mathbf{w}))} \\ &= \ln \int d\mu(\mathbf{w}) e^{n\beta} e^{-n\beta\epsilon(\mathbf{w})} \\ &= \ln \left( \int d\mu(\mathbf{w}) e^{n\beta} \right) + \ln \left( \int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})} \right) \\ &= \ln e^{n\beta} + \ln \left( \int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})} \right) \\ &= n\beta - \beta F_n^{ST} \end{aligned} \quad (63)$$

1372 Dividing by  $n$ , we can also recover the more general relation for the *Average* Free Energy,  $\bar{\Gamma}_{\bar{Q}} =$   
 1373  $1 - \bar{F}_n$ . (Eqn. 38). For the matrix case we do something similar; see Appendix A.3.

1374 Likewise, one can show that the Quality  $\bar{Q}$  (again, always in the AA and at high-T) can be  
 1375 identified as the Thermal Average of the (data-averaged or Annealed) Self-Overlap,

$$\bar{Q} = \left\langle \langle \eta(\mathbf{w}, \xi) \rangle_{\xi^n} \right\rangle_{\mathbf{w}}^\beta = \langle \eta(\mathbf{w}) \rangle_{\mathbf{w}}^\beta \quad (64)$$

1376 We can then obtain  $\bar{Q}$  by taking the appropriate partial derivative of its Generating Function,  
 1377  $\Gamma_Q$ .

1378 For technical reasons, however, we will actually define and use a Generating Function for the  
 1379 Average Layer Quality-Squared  $\bar{Q}^2$ , denoted  $\beta\Gamma_{\bar{Q}^2}^{IZ}$ . In analogy with Eqns. 51 and 52, and at  
 1380 high-T and Large- $\mathcal{N}$  (explained below), we can obtain  $\bar{Q}^2$  (see Section 5 Eqn. 128) as

$$\bar{Q}^2 := \frac{1}{\beta} \frac{\partial}{\partial n} \beta\Gamma_{\bar{Q}^2, N \gg 1}^{IZ} \underset{\text{high-T}}{\approx} \frac{1}{n} \frac{\partial}{\partial \beta} \beta\Gamma_{\bar{Q}^2, N \gg 1}^{IZ} \quad (65)$$

1381 See Section 5 and Appendix A.3 for more details.

#### 1382 4.2.7 The Thermodynamic limit

1383 In the SMOG, the Thermodynamic limit is expressed as the limit of the number of free parameters  
 1384  $m$  grows arbitrarily large,  $m \gg 1$ , but also holding the feature load  $n/m$  fixed (i.e., see [8]). In  
 1385 these older approaches, one is interested in how the thermodynamic properties depend on the  
 1386 feature load. Here, however, we are interested in estimating the generalization accuracy, so we  
 1387 are interested how the thermodynamic properties vary with  $n$ , the number of training examples.  
 1388 For that reason, we will express the Thermodynamic limit as the Large- $\mathcal{N}$  limit in  $n$ . i.e., while  
 1389  $n$  grows arbitrarily large,  $n \gg 1$ , while implicitly fixing the corresponding feature load ( $n/m$  for  
 1390 the ST Perceptron, and  $n/N$  for our ST matrix model, below).



1391 To express the average Free Energy  $\bar{F}_n$  in the Large- $\mathcal{N}$  limit in  $n$ , we can write

$$-\beta\bar{F}_n = \lim_{n \gg 1} \frac{1}{n} \ln \int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})}. \quad (66)$$

1392 When this Large- $\mathcal{N}$  approximation is well behaved, then the total energy  $\mathcal{E}(\mathbf{w})$  is extensive, i.e.,  
 1393 when  $\mathcal{E}(\mathbf{w}) = n\epsilon(\mathbf{w})$ ; and, consequently, the total Free Energy is also extensive, i.e.,  $F_n = n\bar{F}_n$ .  
 1394 This property is a cornerstone of statistical mechanics, as it allows for meaningful macroscopic  
 1395 predictions from microscopic interactions.

1396 **Self-Averaging.** The existence of the limit signifies that the system is *Self-Averaging*, meaning  
 1397 that the macroscopic properties are independent of fluctuations, etc. This also implies that the  
 1398 relevant averages (i.e., training and generalization errors) are the same for almost all samples, or  
 1399 *realizations of the disorder*. Additionally, the Annealed and the Quenched averages,  $\ln\langle Z_n \rangle_{\xi^n}$  and  
 1400  $\langle \ln Z_n \rangle_{\xi^n}$ , respectively, become sharply peaked, and

$$\langle \ln Z_n \rangle_{\xi^n} \approx \ln\langle Z_n \rangle_{\xi^n}, \quad \text{as } n \gg 1 \text{ (grows arbitrarily large)}. \quad (67)$$

1401 For a NN, Self-Averaging implies that the weights  $\mathbf{w}$  are *typical* of the distribution, and therefore  
 1402 the NN can generalize to similar but unseen test examples.

1403 **The Saddle Point Approximation (SPA).** In StatMech, one is frequently faced with in-  
 1404 tractable integrals, and one common solution is to apply Saddle Point Approximation (SPA).  
 1405 The SPA is a Large- $\mathcal{N}$  approximation and is used to describe the system interactions at Large-  
 1406  $\mathcal{N}$ , forming the average or mean interaction over the data. For example, when considering the  
 1407 Large- $\mathcal{N}$  in  $n$  case, we could write

$$\int d\mu(\mathbf{w}) e^{-n\beta\epsilon(\mathbf{w})} \approx \sqrt{\frac{2\pi}{n\epsilon''(\mathbf{w}^*)}} e^{-n\beta\epsilon(\mathbf{w}^*)}, \quad \text{as } n \gg 1 \quad (68)$$

1408 where  $\mathbf{w}^*$  satisfies the saddle point equations:

$$\epsilon(\mathbf{w}^*) := \frac{\partial}{\partial \mathbf{w}} \epsilon(\mathbf{w})|_{\mathbf{w}=\mathbf{w}^*} = 0 \quad (69)$$

$$\epsilon(\mathbf{w}^*) := \frac{\partial^2}{\partial^2 \mathbf{w}} \epsilon(\mathbf{w})|_{\mathbf{w}=\mathbf{w}^*} > 0. \quad (70)$$

1409 These equations guarantee that the solution  $\epsilon(\mathbf{w}^*)$  is at a (local) minimum in  $\mathbf{w}$ . The SPA can  
 1410 be applied to many Large- $\mathcal{N}$  integrals, as long as the integrand decays exponentially,

1411 **Wick Rotation.** When working with complex oscillatory integrands, i.e.,  $e^{iNf(x)}$ , the SPA is  
 1412 frequently combined with a *Wick rotation*, which is used to convert an oscillatory integral to  
 1413 an exponentially decaying one. The Wick rotation is an analytic continuation that rotates the  
 1414 integration variable by 90 degrees, i.e.,  $x \rightarrow \pm ix$ , deforming the integration contour to pass through  
 1415 a saddle point of the integrand:

$$x \rightarrow ix, \quad e^{iNf(x)} \rightarrow e^{-Nf(ix)}, \quad (71)$$

1416 This is typically used in a formal sense; that is, one assumes the resulting complex integrand  
 1417 is both analytic and well-behaved. One would then apply the SPA in the Large- $\mathcal{N}$  in  $N$  case.  
 1418 Below, we will do just this, and use the SPA with a Wick Rotation in both Appendices A.4 and  
 1419 A.6.

**When the Thermodynamic limit fails: atypical behavior.** When the Thermodynamic limit fails to exist, the Free Energy will contain additional, non-extensive terms, i.e.,  $F = n\bar{F}_{ex} + n^{1+x}\bar{F}_{non-ex}$ ,  $x > 0$ .<sup>26</sup> In this case, the AA may fail, the SPA may not apply, and the system may fail to be Self-Averaging. This causes the system to behave in an atypical way, possibly converging to a meta-stable and/or glassy phase. Indeed, when the weights  $\mathbf{w}$  are *atypical*, they may describe the training data well, but they would fail to describe the test data well; in this sense, we say the model is *overfit* to the training data. We will not explicitly consider a model that is non-extensive; however, we will present empirical results where we suspect the model is overfit (in Section 6.5) and, additionally, where we observe glassy behavior, which we refer to as a *Hysteresis Effect* (in Section 6.6).

#### 4.2.8 From the ST Perceptron to a Matrix Model.

In Section 5, we will move from a single  $m$ -dimensional Perceptron vector  $\mathbf{w}$  to a matrix model of  $N \times M$  weights, which can be thought of as  $N$  interacting (feature) vectors of dimension  $M$ . Moreover, in the Student-Teacher (ST) model used below, in the vector case, the  $m$  free parameters (o.e., degrees of freedom) of the feature vectors are integrated out, whereas for the matrix case, we will retain a *reduced set* of the  $M$  degrees of freedom,  $\tilde{M}$ . To do this, we need to ensure the Free Energies and related quantities like the Layer Quality-Squared scale properly.

SETOL uses two Large- $\mathcal{N}$  approximations, the Thermodynamic limit, which is a Large- $\mathcal{N}$  limit in  $n$ , and the *Wide Layer limit*, which is a Large- $\mathcal{N}$  limit in  $N$ :

- Thermodynamic limit:  $m \gg 1$  (the number of parameters or features, fixed load:  $n/m = 1$ )
- Large- $\mathcal{N}$  limit in  $n$ :  $n \gg 1$  (the number of training examples, fixed load:  $n/m = 1$ )
- Wide Layer limit:  $N \gg 1$  (the number of feature vectors,  $n/N$  fixed)

Note that by “limit” we mean  $n$  or  $N$  simply grows arbitrarily large. In taking the Wide Layer Large- $\mathcal{N}$  limit in  $N$ , we assume implicitly that the *layer load*,  $n/N$ , the number data points per feature vector or output dimension  $N$ , remains constant.<sup>27</sup> In doing this, we expect the matrix-generalized total Energies ( $F, H^{an}, \dots$ ) to be Size-Extensive in  $n$  and  $N$ , the average quantities to be Size-Intensive in both, and, as discussed below, *Size-Consistent* in  $\tilde{M}$ .

**Size-Consistency.** The notion of *Size-Consistency* is a notion commonly used Quantum Chemistry to describe interacting, correlated systems. It is often introduced through the Linked Cluster Theorem [49, 98], which states that the *average* energies and/or free energies ( $\bar{F}$ ) of, in particular, a correlated system scale with  $\tilde{M}$ , the number of *independent interacting components*:

$$\begin{aligned} -\beta\bar{F} &= \langle \ln Z \rangle_{\xi^n} = \sum_{\mu=1}^{\tilde{M}} (\text{Connected Components}) \\ &= \sum_{\mu=1}^{\tilde{M}} \text{Cumulants}(\mu) + \text{higher order terms} \end{aligned} \quad (72)$$

For SETOL, below, these connected components will be the matrix-generalized cumulants from RMT. In Quantum Chemistry, this is analogous to ensuring the renormalized Self-Energy and/or Effective Hamiltonian is Size-Consistent. For NNs, Size-Consistency appears when scaling the

<sup>26</sup>When dealing with matrix integrals (below),  $F \sim nNM F_0 + \dots$ , when there are  $n \times N \times M$  degrees of freedom [96].

<sup>27</sup>Although we do not enforce this explicitly here, we note that the so-called “Chinchilla Scaling Law” demonstrates an explicit compute-optimal frontier [97], which we can expect practitioners will likely adhere to.

number of feature vectors  $N$  in our matrix model, and it ensures that our layer Free Energy, etc., remain well-behaved as we increase  $\tilde{M}$ . For a simple example, see Appendix A.2 where we derive the expression for the matrix-generalized Annealed Hamiltonian  $H^{an}$ . Both Size-Extensivity (in  $n$  and  $N$ ) and Size-Consistency (in  $\tilde{M}$ ) are crucial in our SETOL analysis: they justify taking the Large- $\mathcal{N}$  approximation for matrix integrals, and they ensure our resulting HCIZ integral—a sum of integrated RMT cumulants (below)—scales with the dimension of the Effective Correlation Space (ECS),  $\tilde{M}$ .

**HCIZ Integrals** To generalize the Linear ST Perceptron (in the AA, and at high-T) from Perceptron vectors to MLP matrices, we need to generalize the thermal average over the  $m$ -dimensional Perceptron weight vectors ( $\mathbf{w} = \mathbf{s}$ ) to an integral over NN Student  $N \times M$  weight matrices ( $\mathbf{W} = \mathbf{S}$ ). The resulting Partition Function and Free Energy will be expressed with what is called an HCIZ integral. (See Tanaka [83, 84], Gallucio et al. [40] and/or Parisi [96], and also Eqn. 129 in Section 5.) As in Eqn. 14, we will define a *Layer Quality Generating Function*,  $\beta\Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}$ , for the Layer Quality (squared). This will take the form of an HCIZ integral,

$$\beta\Gamma_{\tilde{\mathcal{Q}}^2, N \gg 1}^{IZ} := \lim_{N \gg 1} \frac{1}{N} \ln \underbrace{\int d\mu(\mathbf{A}) \exp[n\beta N \text{Tr}[\mathbf{A}_N \mathbf{X}_N]]}_{\text{HCIZ Integral}} \approx n\beta \text{Tr}[\mathcal{G}_A(\lambda)], \quad (73)$$

that is evaluated in the Wide Layer *Large- $\mathcal{N}$  limit in  $N$*  (here, meaning as  $N \gg 1$ , but not at the limit  $N = \infty$ ). Here,  $\mathbf{A}_N$  and  $\mathbf{X}_N$  are  $N \times N$  Hermetian matrices, (See Appendix A.1 for notation,)  $d\mu(\mathbf{A})$  is a measure over all random (Orthogonal) matrices (see Eqn. 256), and  $\mathcal{G}_A()$  is called a Norm Generating Function (which are different from  $\Gamma_n$ , above, and will be made clear in Section 5.4), defined in Eqn. 132 in Section 5. In applying this, we will actually write  $\text{Tr}[\mathbf{A}\mathbf{X}] = \frac{1}{N} \text{Tr}[\mathbf{A}\mathbf{W}\mathbf{W}^\top] = \frac{1}{N} \text{Tr}[\mathbf{W}^\top \mathbf{A}\mathbf{W}]$ , where  $\mathbf{W}$  is an  $N \times M$  layer weight matrix, and  $\mathbf{A} = \mathbf{A}_N := \frac{1}{n} \mathbf{S}\mathbf{S}^\top$  is an (Outer) layer Correlation matrix, and here,  $\mathbf{X} = \mathbf{X}_N = \frac{1}{N} \mathbf{W}\mathbf{W}^\top$ . Moreover, to evaluate this, we will need to restrict  $\mathbf{A}$  (and  $\mathbf{X}$ ) to the lower-rank Effective Correlation Space (ECS), i.e.,  $\mathbf{A} \rightarrow \tilde{\mathbf{A}}$ . ( $\mathbf{X}$  is already restricted to the span of  $\tilde{\mathbf{X}}$  by ECS assumption.)

Notice that this looks similar to a Saddle Point Approximation (SPA), but where the more complicated function  $\mathbb{G}_{\mathbf{A}}()$  now appears. Also,  $\mathbb{G}_{\mathbf{A}}()$  here depends only on the limiting form of the ESD of  $\mathbf{A}$ ,  $\rho_A^\infty(\lambda)$ , and depends on the  $M$  normalized eigenvalues  $\lambda_i$  of  $\mathbf{X}$ .

To evaluate this, we will form the Large- $\mathcal{N}$  limit in  $N$ , using a result from Tanaka [83, 84], but slightly extended (in Appendix A.6) to include the term  $n\beta$  explicitly. We can write

$$\beta\Gamma_{\tilde{\mathcal{Q}}^2, N \gg 1}^{IZ} := \lim_{N \gg 1} \beta\Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}, \quad (74)$$

with the final result

$$\beta\Gamma_{\tilde{\mathcal{Q}}^2, N \gg 1}^{IZ} = n\beta \sum_{i=1}^{\tilde{M}} \int_{\tilde{\lambda}_{min}}^{\tilde{\lambda}_i} dz R(z), \quad (75)$$

where  $R(z)$  is a complex function, the R-transform of the ESD  $\rho(\lambda)$  of the Teacher, and  $\tilde{\lambda}_i$  are the eigenvalues of Teacher Correlation Matrix  $\tilde{\mathbf{X}}$ , restricted to the ECS. For more details, see Section 5 and Appendices A.4 and A.6.

**Branch Cuts and Phase Behavior.** Free energies ( $F, \Gamma$ ) often exhibit *branch cuts* when expressed as analytic functions of complex parameters (i.e., temperature, coupling constants, or eigenvalue cutoffs), and arise from singularities in the underlying integral representations of the

partition function  $Z_n$ , When a branch cut occurs, this demarcates non-analytic behavior and this indicates the onset of a *phase transition* where macroscopic observables such as correlation lengths and/or variance-like quantities may diverge or change character abruptly.

In the context of our HCIZ-based construction, integrating a complex function like the  $R(z)$ -transform of a Heavy-Tailed ESD can produce precisely this phenomenon. For example, if  $R(z)$  has a square-root term, i.e.,  $(\sqrt{z-c})$ , then it will have a branch cut at  $z=c$ , and the Generating Function (i.e., negative Effective Free Energy)  $\beta\mathbf{T}_{\bar{Q}^2, N \gg 1}^{IZ}$  will be non-analytic and we must choose the appropriate, physically meaningful branch, i.e.,  $(\Re[z] > \tilde{\lambda}_{min})$ , corresponding to the ECS (where  $\Re[z]$  is the Real-part of  $z$ ) We argue that this cut signifies a *phase boundary*—an abrupt change in the system’s correlation structure and corresponds to an emerging singularity in the Layer Quality. Even though we perform only a single exact RG step, (rather than fully iterating a renormalization flow), the appearance of a branch cut in  $\beta\mathbf{T}_{\bar{Q}^2, N \gg 1}^{IZ}$  will encode nontrivial *phase-like* behavior in the SETOL Heavy-Tailed matrix model.

### 4.3 Student-Teacher Perceptron

In this subsection, we present a unified view of the *Student-Teacher* (ST) Perceptron model from both a practical and a theoretical perspective. The common sense modern understanding of Student-Teacher learning typically involves knowledge distillation: a larger, pretrained neural network (the *Teacher*) is used to train a smaller network (the *Student*), which learns to imitate the Teacher’s outputs  $y_\mu^T$ . In practical terms, this often helps the smaller Student achieve comparable performance more efficiently [99]. And it remains an open question as to why this works so well. In contrast, classical theoretical models from the Statistical Mechanics of Generalization (SMOG) interpret the Student-Teacher relationship differently. Here, the Teacher is an idealized theoretical model  $T$ , a Perceptron (vector)  $\mathbf{t}$ , that explicitly generates (binary) labels  $y_\mu^T$  from some idealized data  $\xi$ , and the Students  $S$  are Perceptrons (vectors) of the same size as the Teacher,  $\|\mathbf{s}\| = \|\mathbf{t}\|$ , selected from a Boltzmann distribution. The ST theory seeks simple analytic derivations of the generalization errors  $\bar{\mathcal{E}}_{gen}^{ST}$  under different simplifying assumptions (AA, high-T, linear activations, etc.), in order to understand phenomena such as what is now called Double Descent[100], NN storage capacity, learning with noisy labels, memorization vs. generalization, and other fundamental learning phenomena[18, 101, 4, 102, 7, 8]. A key result is that  $\bar{\mathcal{E}}_{gen}^{ST}$  is a simple analytic function of the ST *Overlap*,  $R = \mathbf{s}^\top \mathbf{t}$ . Our SETOL approach is motivated by both these perspectives, and introduces a novel, Semi-Empirical twist. We seek a matrix-generalization of the classical vector ST model. And while inspired by the ST Perceptron, rather than an idealized theoretical Teacher  $T$ , we take the Teacher as an empirical input—a layer weight matrix,  $\mathbf{T} = \mathbf{W}$ , taken from a real model—a model you might train yourself, download, or acquire elsewhere. We aim to estimate the layer accuracy (or precision), which we call Layer Quality  $\bar{Q}$ , using an ensembles of similar Students,  $S \sim T$ , i.e.  $N \times M$  matrices,  $\mathbf{S}, \mathbf{T}$ .  $\bar{Q}$  is also a function of the ST Overlap, now a matrix,  $\mathbf{R} = \frac{1}{N} \mathbf{S}^\top \mathbf{T}$ , but now also critically depends on the ESD of  $\mathbf{T}$ . And while our Students are the same size as the Teacher, we will find later that the optimal Teacher is actually much smaller than the one we started out with.

**Practical framing.** Imagine being a real-world practitioner who has trained a large-scale neural network (NN), or downloaded it from the internet, or received it by other means — an increasingly common scenario. We call this NN the Teacher, because it is the primary empirical input to the theory. The term “Teacher” means that we consider this object to be the original source of supervision – this trained model replicates the training labels  $y_\mu^T$ , often to perfection

(interpolation) or nearly so.<sup>28</sup> You also hold a dataset  $\mathbf{D}$  that approximates the distribution on which  $T$  was trained, yet you lack a reliable yardstick for evaluating  $T$ 's outputs: perhaps  $\mathbf{D}$  is contaminated with test data, or  $T$  is an LLM with highly arbitrary outputs, or you just don't have access to test data. In any case, you can escape this bind by applying a *Student-Teacher* protocol. You retrain one or more Students  $S_1, S_2, \dots$  on  $\mathbf{D}$  using ordinary tools (SGD), that resemble the Teacher  $T$  (same size, amount of regularization, etc), but now slightly varying the training procedures (i.e., initial conditions, optimization hyperparameters, etc.)—tasking them solely with *imitating*  $T$ 's predictions. Averaging over many such Students, you can obtain an *indirect but quantitative* estimate of  $T$ 's performance.

**Why this works.** We view  $T$  as an *inevitable* outcome of the training pipeline: if you reran the same recipe many times, you would likely converge on a narrow family of similar models. The tighter that distribution, the more *Precise* it is, and—assuming the ground-truth concepts  $y_\mu^T$  are at least *nearly* realizable—the closer any single draw (your Teacher) must sit to the truth. By comparing Student and Teacher outputs, you can approximate the Teacher's generalization performance even without an explicit hold-out set. Notably, if the Teacher perfectly interpolates its training data, the Student's error directly estimates the Teacher's *true* Generalization Accuracy. Otherwise, it captures the Teacher's *Precision* in reproducing its own noisy or biased labels.

**An extended theory.** We seek a succinct, analytic formulation of the ST Average Generalization Error, denoted  $\bar{\mathcal{E}}_{gen}^{ST}$ . We work in the Annealed Approximation (AA) – a simplification often valid when networks are sufficiently large and can nearly interpolate their training data. Under this approximation, one obtains closed-form expressions for the Student-Teacher *Overlap* ( $R$ ) and thus for the Teacher overall error or accuracy. Take note also that we do not assume that the labels  $y_\mu^T$  are realizable by the Teacher, but, rather, take the Teacher as empirical input to the theory. This point is both subtle – since the derivations proceed closely at times to those found in [91, 102, 7, 8] – and also radical, because our derived quality metrics  $\bar{\mathcal{Q}}$  now depend directly on empirical properties of the Teacher. These results lay the foundation for our *Semi-Empirical* approach, in which we supplement this theoretical form with empirical measurements (e.g., from the trained weight matrices) to account for real-world correlations in the data and the model's internal structure. **As far as we know, this is completely new Semi-Empirical approach for modeling NNs.**

**4.3.1 Operational Setup.** In subsection 4.3.1 we explain how to set up our formulation Student-Teacher model in an *operational* manner. In particular, we emphasize the difference between *true accuracy* (vs. ground-truth labels) and Precision (vs. the Teacher's own labels). We also discuss the difference between our Quality metrics and the *Generalization Gap*.

**4.3.2 Theoretical Student-Teacher Average Generalization Error ( $\bar{\mathcal{E}}_{gen}^{ST}$ ).** In subsection 4.3.2 we outline how to derive  $\bar{\mathcal{E}}_{gen}^{ST}$  using the AA. We introduce the key expressions that will serve as the starting point for our extended Semi-Empirical theory in subsequent subsubsection.

### 4.3.1 Operational Setup

Here, describe the basic setup of the classic Student-Teacher model, taking an operational view from the perspective of a practitioner training real-world Student and Teacher models. Specifically, we present the Annealed Approximation (AA) in a practical light, and use it to explain the

<sup>28</sup>If nearly so, then we consider this label noise to be the contribution of the Teacher, which SETOL can characterize.

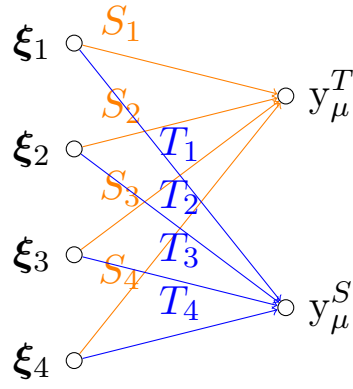


Figure 8: Pictorial representation Student and Teacher Perceptrons.

1575 difference between computing the *Empirical Generalization Error*,  $\bar{\mathcal{E}}_{gen}^{emp}$ , for the *True Accuracy*  
 1576 and for the *Precision* of a Teacher model. Table 6 summarizes some of the key notation we will  
 be using in this section, and also the next two sections for reference.

Symbol	Meaning
$T$	Teacher model (fixed network)
$S$	Student model (trained to mimic $T$ )
$\mathbf{D}$	True dataset of $(\mathbf{x}_\mu, y_\mu^{true})$ pairs
$\mathcal{D}$	Gaussian-field idealization of $\mathcal{D}$
$\bar{\mathcal{E}}_{gen}^{emp}$	Average empirical test-set error estimate
$\bar{\mathcal{E}}_{gen}^T$	Average, true generalization error of $T$ (unknown)
$\bar{\mathcal{E}}_{gen}^{ST}$	Student–Teacher average generalization error
$\mathbf{s}, \mathbf{t}$	Student and Teacher weight vectors
$y_\mu^S, y_\mu^T$	Student and Teacher labels (+1 −1) for example $\mu$
$R$	Student-Teacher Overlap $R = \mathbf{s}^\top \mathbf{t}$
$\epsilon(R)$	Annealed Error Potential (i.e., $1 - R$ )
$\eta(\mathbf{s}, \mathbf{t})$	Self-Overlap (i.e., $R$ )
$\bar{Q}^{ST}$	Student-Teacher Perceptron Quality

Table 6: Key notation for our formulation of the Student–Teacher model.

1577

1578 **Test Error of the Teacher.** We start by describing how to obtain a simple formal expression  
 1579 for the empirical test errors of the Teacher  $T$ . Let us say we have a model, called Teacher ( $T$ ),  
 1580 which maps some *actual* (i.e., correlated, meaning the features are not i.i.d.) data  $\mathbf{x}_\mu \in \mathbf{D}$  to some  
 1581 known or *true* labels ( $y_\mu^{true}$ ) (where,  $y_\mu^{true}$  is, say, an  $N$ -dimensional vector of binary labels). We  
 1582 might say that  $y_\mu^{true}$  represents the *Ground Truth* for the problem. Operationally, we train the  
 1583 Teacher  $T$  to reproduce or at least approximate the true labels  $y_\mu^{true}$ .

$$T : \mathbf{x}_\mu \rightarrow y_\mu^T \approx y_\mu^{true}. \quad (76)$$

1584 If  $T$  reproduces the true labels exactly, we might say that the Teacher has been trained to  
 1585 *Interpolation*, and therefore,  $y_\mu^T = y_\mu^{true}$ . Indeed, most models today are trained to *Interpolation*,  
 1586 and we don’t need to necessarily worry about the difference between the true and the predicted



1587 Teacher labels. Formally, however, and to better understand the AA, it is beneficial to discuss  
 1588 the implications of this distinction.

1589 Following Eqn. 1, let's say the Teacher outputs are specified by the NN output (or inference  
 1590 energy) function  $E_{NN}^{out}$ <sup>29</sup>

$$y_{\mu}^T = E_{NN}^{out}(T, \mathbf{x}_{\mu}) \quad (77)$$

1591 so that we may write the *Empirical Average Training Error*  $\bar{\mathcal{E}}_{train}^{emp}$  as

$$\bar{\mathcal{E}}_{train}^{emp} := \frac{1}{N^{train}} \sum_{\mu=1}^{N^{train}} \mathcal{L}[y_{\mu}^{train}, E_{NN}^{out}(T, \mathbf{x}_{\mu}^{train})]. \quad (78)$$

1592 Ideally, we seek the *True Average Generalization Error* of the Teacher, denoted  $\bar{\mathcal{E}}_{gen}^T$ . Of course,  
 1593 this is unknowable, but in practice, we estimate  $\bar{\mathcal{E}}_{gen}^T$  by measuring the error of the Teacher  
 1594 predictions on some test (or hold-out) set  $(\mathbf{x}_{\mu}^{test}, y_{\mu}^{test})$ . We call this the *Empirical Average Gen-*  
 1595 *eralization Error*,  $\bar{\mathcal{E}}_{gen}^{emp}$ , and write

$$\bar{\mathcal{E}}_{gen}^T \approx \bar{\mathcal{E}}_{gen}^{emp} := \frac{1}{N^{test}} \sum_{\mu=1}^{N^{test}} \mathcal{L}[y_{\mu}^{test}, E_{NN}^{out}(T, \mathbf{x}_{\mu}^{test})]. \quad (79)$$

1596 To measure the error, the loss function  $\mathcal{L}$  may be an L1 ( $\ell_1$ ) or L2 ( $\ell_2$ ) loss; whereas for training  
 1597 a NN model, it is usually something like a cross-entropy loss.<sup>30</sup>

1598 If we don't have a hold-out set, however, we can still estimate  $\bar{\mathcal{E}}_{gen}^T$  using the Student-Teacher  
 1599 approach.

1600 **Estimating the Student-Teacher Error: Accuracy vs. Precision.** Imagine we train a  
 1601 Student model  $S$  (with the same architecture as the Teacher  $T$ ) on the real-world dataset  $\mathbf{D}$ ,  
 1602 using  $T$ 's outputs as targets:

$$S : \mathbf{D} \rightarrow y_{\mu}^S \approx y_{\mu}^T,$$

1603 where  $y_{\mu}^T = E_{NN}^{out}(T, \mathbf{x}_{\mu})$  are the Teacher's predicted labels or energies.

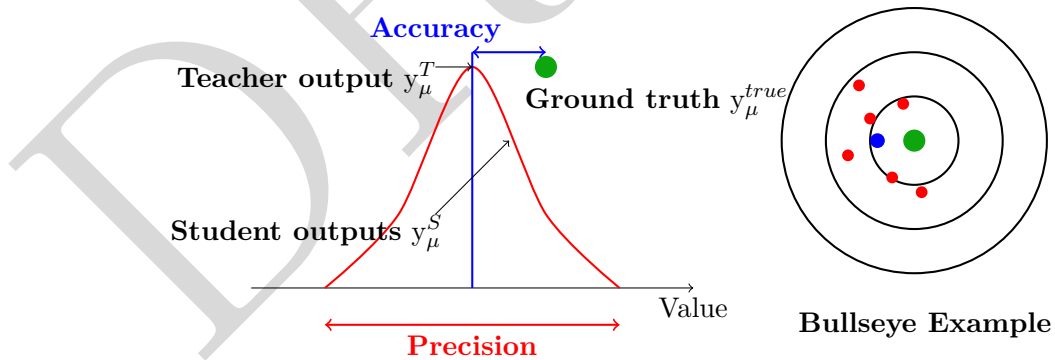


Figure 9: Precision vs. Accuracy

1604 Figure 9 illustrates the following two scenarios side by side:

<sup>29</sup>We refer to outputs of  $E_{NN}^{out}(\mathbf{t}, \mathbf{x}_{\mu})$ , when applied to a data point  $\mathbf{x}_{\mu}$ , as energies because they are effectively un-normalized probabilities for the class outputs (for labels  $y_{\mu} = 1$  or  $-1$ ).

<sup>30</sup>Note that  $\bar{\mathcal{E}}_{gen}^T$  will be treated as an energy function, as is  $E_{NN}^{out}$ , yet they are related nonlinearly. This is because they are energies in *two different systems* – training, and inference – and  $\mathcal{L}$  is a transfer function that bridges them.

- **Accuracy (Interpolation) regime:** If  $T$  perfectly interpolates the true labels ( $y_\mu^T = y_\mu^{\text{true}}$ ), then  $\|y_\mu^S - y_\mu^T\| = \|y_\mu^S - y_\mu^{\text{true}}\|$  measures how well the student recovers the Ground Truth labels—i.e., the Student’s *training accuracy*.
- **Precision (Noisy teacher) regime:** If  $T$  itself makes mistakes ( $y_\mu^T \neq y_\mu^{\text{true}}$ ), then  $\|y_\mu^S - y_\mu^T\|$  estimates how faithfully  $S$  reproduces  $T$  (its precision), rather than true accuracy.

By analyzing the Student–Teacher overlap  $R = \sum_\mu s^\top t$ , one can show that the average generalization error of  $T$  depends simply on  $1 - R$  under the annealed approximation—even when  $T$  was trained on noisy labels. In practice, we exploit this fact by training a large ensemble of students to estimate  $R$  and hence recover the teacher’s true error.

The Student–Teacher model also explains why NNs can generalize even when trained to Interpolation on noisy data (which has been a source of confusion [103]). In this model, the Generalization Error  $\bar{\mathcal{E}}_{\text{gen}}^T$  is a simple function of the overlap  $R$  between the Teacher  $T$  and the Students  $S$ , i.e.,  $\bar{\mathcal{E}}_{\text{gen}}^T \sim \langle 1 - \epsilon(R) \rangle_s^\beta$ . So even if the Teacher  $T$  is trained on noisy data, as long as there are Students  $S$  with significant overlap  $R$  with the Teacher, the Teacher Generalization Error  $\bar{\mathcal{E}}_{\text{gen}}^T$  can be considerably small. For more details, see [104].

**Learning the Student.** Moving forward, we will always assume the Teacher is trained to Interpolation because this actually corresponds to the Annealed Approximation, whereas if the Teacher makes errors, we may need to consider Quenched averages, explained below.

Imagine now that to estimate the empirical Average Generalization Error,  $\bar{\mathcal{E}}_{\text{gen}}^{\text{emp}}$ , by training a very large number of Students, and computing the average ST error on some test set. Let us break the data set into training  $\mathbf{x}_\mu^{\text{train}}$  and test  $\mathbf{x}_\mu^{\text{test}}$  examples, train models on the training data (that is, find the optimal model weights), and evaluate the  $S$  and  $T$  models on the test data.

The Student learning task can be written as in Eqn. (2) as the following optimization problem over the training data:

$$\operatorname{argmin}_{\{S'\}} \sum_{\mu=1}^{N^{\text{train}}} \mathcal{L}[E_{\text{NN}}^{\text{out}}(S', \mathbf{x}_\mu^{\text{train}}), E_{\text{NN}}^{\text{out}}(T, \mathbf{x}_\mu^{\text{train}})], \quad (80)$$

If the Teacher is trained to Interpolation, then the NN optimization problem training a Student to reproduce the Ground Truth labels, so that  $y_\mu^S \sim y_\mu^{\text{true}}$  for both the training and test sets.

$$\operatorname{argmin}_{\{S'\}} \sum_{\mu=1}^{N^{\text{train}}} \mathcal{L}[E_{\text{NN}}^{\text{out}}(S', \mathbf{x}_\mu^{\text{train}}), y_\mu^{\text{true}}], \quad (81)$$

If not, then the Student is reproducing the possibly incorrect Teacher labels, and, importantly, the Student  $S$  now depends explicitly on how the Teacher was trained. That is, we should denote that the learned Student explicitly depending on  $T$ , i.e.  $S \rightarrow S[T]$ . This will be important below.

**The Thermal Average.** In StatMech, the average over Student weights  $\langle \dots \rangle_s$  is a Thermal Average  $\langle \dots \rangle_s^\beta$ . This means we should restrict the choice of  $S$  to the same Boltzmann distribution we assume  $T$  is drawn from. In a practical sense, we would expect our Students  $S$  to be trained with the roughly same amount of regularization (same weight decay, etc.). In principle, we should be able to admit many kinds of  $S$ , including those arising from different optimization paths which lead to the same equilibrium sample.<sup>31</sup> While the parameter  $\beta$  is like a fixed regularization set-

<sup>31</sup>See [105], which shows that for NNs trained with SGD, nearly all learning rates, if they are not too large, converge to the same minima given enough time. Additionally, [106] shows that one can effectively train with any batch size and learning rate—as long as you schedule them correctly (i.e., growing them)—and still guarantee convergence to the same solution.

ting, it actually modulates the trade-off between energy and entropy— sometimes called *entropic regularization*—and therefore how strongly the data constrains the model, and not specifically how the model is trained. Moreover, in the high- $T$  (small- $\beta$ ) limit the measure becomes broader, so we can admit more Student weights that fluctuate around the mean. In practice, however, we find that different optimizer settings (batch sizes, learning rates, stopping criteria, etc.) can give very different results. Therefore, we must be careful not to admit any arbitrary Student into the average because this would amount to averaging over *several* Boltzmann distributions and this should be treated explicitly.

**The Average Generalization Error.** We may seek to estimate the Empirical Average Generalization Error by replacing the test predictions in Eqn. 79 with the student predictions  $y_\mu^{test} \rightarrow y_\mu^S$ , and then averaging directly over the test data  $\mathbf{x}_\mu^{test}$  for all possible or available test examples.

If we have a very large number of suitable Students (say, drawn from some random distribution), then we can try to estimate the Average Generalization Error of the Teacher, i.e.,  $\mathcal{E}_{gen}^T \approx \bar{\mathcal{E}}_{gen}^{emp}$ .  $\bar{\mathcal{E}}_{gen}^{emp}$  is given by an average loss, the average is over all possible Students  $N_S$ , and then over all  $N^{test}$  test data points  $\mathbf{x}_\mu^{test} \in \mathbf{D}$

$$\begin{aligned}\bar{\mathcal{E}}_{gen}^{emp} &= \frac{1}{N^{test}} \sum_{\mu=1}^{N^{test}} \frac{1}{N_S} \sum_S \mathcal{L}[E_{NN}^{out}(S, \mathbf{x}_\mu^{test}), E_{NN}^{out}(T, \mathbf{x}_\mu^{test})] \\ &= \frac{1}{N_S} \sum_S \frac{1}{N^{test}} \sum_{\mu=1}^{N^{test}} \mathcal{L}[E_{NN}^{out}(S, \mathbf{x}_\mu^{test}), E_{NN}^{out}(T, \mathbf{x}_\mu^{test})],\end{aligned}\tag{82}$$

where (ideally)  $N^{test}$  is extremely large.

In Bra-Ket notation, we may also write

$$\begin{aligned}\bar{\mathcal{E}}_{gen}^{emp} &= \langle \langle E_{\mathcal{L}}^n(S, T, \mathbf{x}) \rangle_S \rangle_{\mathbf{x}^{test}} \\ &= \langle \langle E_{\mathcal{L}}^n(S, T, \mathbf{x}) \rangle_{\mathbf{x}^{test}} \rangle_S\end{aligned}\tag{83}$$

where  $E_{\mathcal{L}}^n(S, T, \mathbf{x}) := \mathcal{L}[E_{NN}^{out}(S, \mathbf{x}_\mu^{test}), E_{NN}^{out}(T, \mathbf{x}_\mu^{test})]$ . For the empirical estimate, it does not matter what order we take the sums in, but we are not estimating the the True Average Generalization Error of the Teacher,  $\bar{\mathcal{E}}_{gen}^T$ , unless  $T$  is trained to Interpolation. For the theoretical estimate, however, the order can be important, and this also depends on if  $T$  is trained to Interpolation or not. <sup>32</sup>

**Annealed vs. Quenched Averages.** Recall that in the StatMech approach to computing errors, we do not break the data into training and test, but, instead, to obtain the Average Generalization Error,  $\bar{\mathcal{E}}_{gen}$ , use the Generating Function approach. In doing this, we need to compute both the Thermal Average over the model weights  $(S, T)$ , and also take the data average over the entire available idealized data set  $\mathcal{D}$ . And the order can matter.

In the case where the Teacher is trained to Interpolation, may train the Student independently of *when* the Teacher. But if Teacher is *not* trained to Interpolation, then formally we must train the Teacher first to obtain target predictions for the Student. That is, the Student formally depends on the Teacher,  $S[T]$ . The empirical errors in  $T$  would then formally depend on the specific instantiation of the data  $\xi^n \in \mathcal{D}$ , and therefore, conceptually imagine that we must first average over the data before averaging over the weights. *Training to Interpolation* corresponds

<sup>32</sup>This approach can be likened to the Bootstrap method [107] used for error estimation. However, the Bootstrap method predominantly emphasizes variations in the input data  $\mathbf{x}^n \in \mathbf{D}$ , while in this context, we are essentially bootstrapping over the students  $S$ .

conceptually to working with a model in the Annealed Approximation, whereas not doing so corresponds to Quenched case.

Practically, when the Teacher is not trained to Interpolation, we may need to resample the training data and training an ensemble of models to compensate for anomalies in training data (bad labels, noise, etc.) that may cause the underlying model to overfit to the training data. Theoretically, within SMOG, this is equivalent to *quenching* the system to the data (a term analogous to quickly cooling a physical system, freezing in any defects). In contrast, when one *anneals* a physical system, one heats up and cools it down slowly, and repeatedly, thereby removing any defects (of data anomalies for NNs, or material defects in a physical system).

In StatMech, one can perform a so-called quenched average using a replica calculation, effectively removing the dependence on test and/or training data from the final estimate for  $\bar{\mathcal{E}}_{gen}^{emp}$ . However, the theoretical quenched result may differ significantly from the annealed case when the underlying model is unrealizable [8]. This may occur when the training data is very noisy and/or the model architecture is such that it can not correctly predict all the training labels. In such cases, the model will always have some finite, non-zero Average Training Error,  $\bar{\mathcal{E}}_{train} > 0$ , even in the Large- $\mathcal{N}$  limit of infinite data  $n = \infty$ . In such a case, this indicates a highly complex error landscape with many local minima separated by extremely high barriers, and a slowing down of the dynamics.<sup>33</sup>

While it is commonplace to train ensembles and/or use cross-validation when training small models (as the above discussion assumes), this could be extremely expensive and impractical in modern ML, e.g., for very large models like Large Language Models (LLMs). For such massive NNs, one needs a theory that can detect anomalies in training directly from observations during and/or after training. This is a hallmark of the SETOL approach, and it distinguishes SETOL from the classic StatMech approach.

**What about Grokking?** There could be a scenario where the Teacher  $T$  is trained to interpolation, achieving perfect training accuracy, and, yet, the test accuracy remains low; This scenario happens in Grokking, in both the *pre-Grokking* and *anti-Grokking* phases, and has been analyzed using the HTSR theory.[108] In the pre-Grokking case, the Teacher has not properly converged, and has one or more layer  $\alpha \gg 2$ , whereas in the anti-Grokking phase, the layers have may be overfit or overcorrecting, with  $\alpha \ll 2$ . In either case, we might argue that Teacher has not achieved Thermodynamic equilibrium, and the ST approach may fail! This complex situation highlights why it is necessary to have a robust theory that can characterize the internal states of the NN layers, and without needing access to test or training data.

**Generalization Gap vs. Model Quality.** We should distinguish between what is typically done in the SLT literature versus the StatMech approaches. In SLT, one is typically interested in modeling the *Generalization Gap*. The Generalization Gap quantifies the difference between a models performance on training data versus unseen test data:

$$\mathcal{E}_{gap}^{emp} := \mathcal{E}_{train}[\mathbf{x}^{train}] - \mathcal{E}_{gen}[\mathbf{x}^{test}] \quad (84)$$

In contrast, in StatMech approaches, one considers the Model Generalization Accuracy directly, which is sometimes called the Model Quality in the SLT literature. Model quality is an indication of the models accuracy, precision, recall, or any other relevant metric based on the task at hand.

While related, in developing an analytic theory, the Generalization Gap and the Model Quality (or Model Generalization Accuracy) require conceptually different approaches. This is because

<sup>33</sup>In modern ML parlance, one might say the model can not be evaluated at interpolation, although in practice such a model might have a zero empirical Training Error since it may overfit the specific training data.

the Generalization Gap depends on a specific realization of the training data, whereas our Model Generalization Accuracy will be formulated on a random training data set (and then corrected later with empirical data). In this sense, any theory of the Generalization Gap requires a formalism where the predicted model error is Quenched to the training data, which is not what we want. In contrast, the Model Generalization Accuracy will be formulated using the Annealed Approximation (AA), and is therefore both conceptually and mathematically simpler. Notably, the HTSR model Quality metric trend well when compared to the Model Generalization Accuracy, whereas methods from the SLT literature tend to only describe the Generalization Gap well.[28]

#### 4.3.2 Theoretical Student-Teacher Average Generalization Error ( $\bar{\mathcal{E}}_{gen}^{ST}$ )

Here, we seek a simple, formal expression for the Student-Teacher Average Generalization Error,  $\bar{\mathcal{E}}_{gen}^{ST}$ , that can be used as the starting point for our extended Semi-Empirical theory.

**The Idealized Data.** To develop a Semi-Empirical theory of the Teacher Generalization Error,  $\mathcal{E}_{gen}^T$ , instead of training and evaluating a NN model using real data ( $\mathbf{x}$ ), we seek a simple, analytical expression with parameters that can be fit to empirical measurements. So in addition to using a model for our NN, we must specify a idealized model for the data. In a real NN, the data  $\mathbf{x}$  is correlated, and, in fact, very strongly correlated; and this is reflected in the layer weight matrices. However, to be tractable, our starting theoretical expressions use uncorrelated (i.i.d) data. Formally, we must replace the correlated data with some uncorrelated, random model of the data, i.e.,  $\mathbf{x} \rightarrow \boldsymbol{\xi}$ . As described in Figure 7, our Data Model is a standard Gaussian  $N(0, \sigma^2 \mathbb{I})$  model for the input data

$$\mathbf{x}_\mu \rightarrow \boldsymbol{\xi}_\mu, \quad \boldsymbol{\xi}_\mu \in N(0, \sigma^2 \mathbf{I}_m), \quad (85)$$

where  $N(0, \sigma^2 \mathbf{I}_m)$  denotes a Gaussian distribution with zero mean and variance  $\sigma^2 = \frac{1}{m}$ ,  $\boldsymbol{\xi}_\mu$  is normalized such that  $\|\boldsymbol{\xi}_\mu\|^2 := \sum_{i=1}^m (\xi_{\mu,i})^2 = 1$  for all  $n$  data vectors. The full idealized sample is denoted  $\boldsymbol{\xi}^n$ , and is an  $n \times m$  matrix, or, equivalently, a  $n$ -dimensional vector of  $m$ -dimensional vectors  $\boldsymbol{\xi}_\mu$ .

We make this distinction between actual  $\mathbf{D}$  and idealized data  $\mathcal{D}$  to emphasize that, later, we will use our so-called Semi-Empirical procedure to account for the real correlations in the actual data phenomenologically by taking some analytical parameter of the theory and fitting it to the real world observations, here, on the ESD of the NN weight matrices.

**The ST Error Model and the Annealed Potential  $\epsilon(\mathbf{s}, \mathbf{t})$ .** We now model Teacher error  $\bar{\mathcal{E}}_{gen}^T$  with the *Average ST Generalization Error*  $\bar{\mathcal{E}}_{gen}^{ST}$ , which is obtained by *first* computing the ST error function  $E_{\mathcal{L}}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n)$  over the set of *all* possible  $n$  input examples  $\boldsymbol{\xi}$ . Define the data-dependent ST test error function—or Energy—as

$$E_{\mathcal{L}}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) := \sum_{\mu=1}^n \mathcal{L}[E_{NN}^{out}(\mathbf{s}, \boldsymbol{\xi}_\mu), E_{NN}^{out}(\mathbf{t}, \boldsymbol{\xi}_\mu)]. \quad (86)$$

where  $\mathcal{L}(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}_\mu)$  is simply the  $\ell_2$  loss. This measures the error between the Student and the Teacher; it is zero when their predictions are identical, ( $y_\mu^S = y_\mu^T$ ), and is nonzero otherwise.

We aim to derive a simple expression for the Average ST Generalization Error,  $\bar{\mathcal{E}}_{gen}^{ST}$ , and to do this, we define the Annealed Error Potential for the data-averaged ST Generalization Error  $\epsilon(\mathbf{s}, \mathbf{t})$ , as in Eqn. 30, as:

$$\epsilon(\mathbf{s}, \mathbf{t}) = \langle E_{\mathcal{L}}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \rangle_{\bar{\boldsymbol{\xi}^n}} := \frac{1}{n} \int d\mu(\boldsymbol{\xi}^n) E_{\mathcal{L}}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \quad (87)$$

The measure  $d\mu(\xi^n)$  will end up being a Gaussian measure over  $n$  samples (see Appendix A.2), and the intent is to evaluate it in the Large- $\mathcal{N}$  limit in  $n$ , thereby sampling all possible inputs in the idealized data space,  $\xi^n \in \mathcal{D}$ .

As in Section 4.2, by applying the AA, we can rewrite the Average ST Generalization Error,  $\bar{\mathcal{E}}_{gen}^{ST}$ : first, a simple average over all the possible inputs  $\xi^n$ ; and, second, then as a Thermal average over all Students  $S$ , in the AA, and at high-T

$$\bar{\mathcal{E}}_{gen}^{ST} := \langle \epsilon(\mathbf{s}, \mathbf{t}) \rangle_{\mathbf{s}}^{\beta}. \quad (88)$$

(Recall that in this regime,  $\bar{\mathcal{E}}_{gen}^{ST} = \bar{\mathcal{E}}_{gen}^{an, hT}$ .)

In the classic **StatMech** approach, the average  $\langle \dots \rangle_{\mathbf{s}}^{\beta}$  is a Thermal Average in the canonical ensemble with  $\beta$  fixed, as explained in Section 4.2. Here, we will do something similar, as the Student average  $\langle \dots \rangle_{\mathbf{s}}^{\beta}$  will be computed from the associated generating function  $\beta \mathbf{\Gamma}_{\mathcal{Q}^2}^{IZ}$  for the matrix-generalized case (an HCIZ integral defined over all students, and in both the Large- $\mathcal{N}$  Thermodynamic limit in  $n$ , and the Wide Layer Large- $\mathcal{N}$  limit in  $N$ ).

Recall that above, the empirical estimate for  $\bar{\mathcal{E}}_{gen}^{emp}$  depended on a specific instantiation of the model for the training data  $\mathbf{x}_{\mu}^{train}$ , i.e.  $\bar{\mathcal{E}}_{gen}^{ST}$  is Quenched to the training data. For that reason, for the final result, we needed to take a second, quenched average over all possible data sets. Here, we do not need to consider this and always work in the Annealed Approximation (AA). This is because we incorporate the specific effects of the real-world training data ( $\mathbf{x}^n$ ) after we derive our formal expressions by fitting the model parameters to empirical data. The final expression for  $\bar{\mathcal{E}}_{gen}^{ST}$ , derived below, will be generalized to  $\bar{\mathcal{E}}_{gen}^{NN}$ , matrix-generalization of the classic **StatMech** formula for the Linear Perceptron, in the Annealed and High-T approximations. (see Appendix A.2).

**The Annealed Potential as a function of the overlap ( $\epsilon(R)$ ).** We want an expression for the data average of the ST test error, from Eqn. 87, generalized from Perceptron vectors to NN layer weight matrices. For the Perceptron, one obtains different expressions for the ST error function, depending on the type of activation function  $h(x)$  in Eqn. 1; The simplest are the Linear and Boolean Perceptrons, and for both (and with  $\ell_2$  loss),  $\epsilon(\mathbf{s}, \mathbf{t})$  is simply a function of the ST overlap  $R$  [8]. This gives  $\epsilon(\mathbf{s}, \mathbf{t}) \rightarrow \epsilon(R)$ , where

$$R = \mathbf{s}^{\top} \mathbf{t} = \sum_{i=1}^m s_i t_i, \quad R \in [0, 1]. \quad (89)$$

which is simply the dot product between the  $m$ -dimensional Student  $\mathbf{s}$  and Teacher  $\mathbf{t}$  weight vectors. Notice that the data vectors are normalized such that  $\|\mathbf{s}\|^2 = \|\mathbf{t}\|^2 = 1$  and we assume there are *no inversely-correlated* Students—Students that predict more than half the Teacher labels incorrectly. And, importantly, the number of free parameters becomes 1.

For a Linear Perceptron [8],<sup>34</sup> with activation function  $h(x) = x$ , we can obtain the error function as

$$\epsilon(R) = 1 - R, \quad R \in [0, 1]. \quad (90)$$

<sup>34</sup>In the classic approach for the ST model, the theory examined different expressions  $\epsilon(R)$ . For example, one can consider the Boolean Perceptron [8, 109], with activation function  $h(x) = \text{sgn}(x)$ , i.e., the Heaviside step function. Then, the error is  $\epsilon(R) = 1 - \frac{1}{\pi} \arccos(R)$ . In both cases, perfect learning occurs when  $R = 1$  [8].



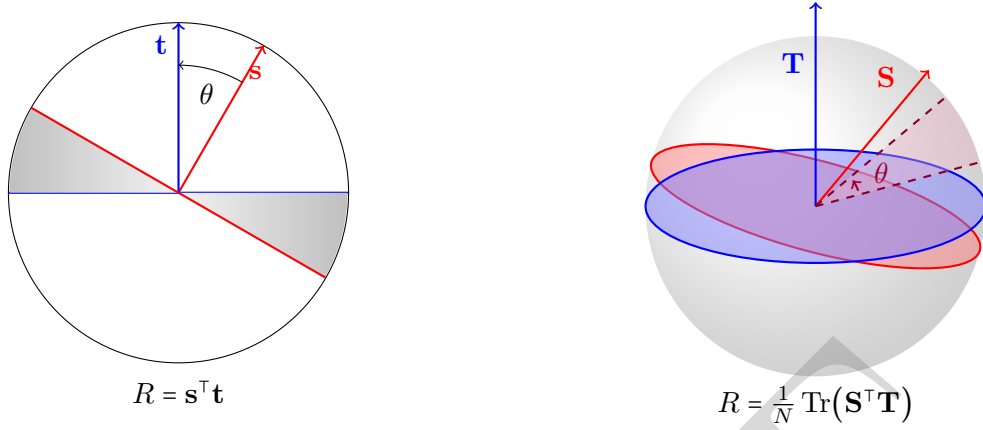


Figure 10: Comparison of 2D and 3D representations of the vector and matrix Student-Teacher overlap  $R$ . **Left:**  $R = \mathbf{s}^\top \mathbf{t}$  (and normalized s.t.  $\|\mathbf{s}\|^2 = \|\mathbf{t}\|^2 = 1$ ). **Right:**  $R = \frac{1}{N} \text{Tr}(\mathbf{S}^\top \mathbf{T})$  with conic sections on the sphere (red  $\mathbf{S}$ , blue  $\mathbf{T}$ ), plus a purple wedge for the angle. Averaged over matrix dimension  $N$  (and implicitly normalized over to  $1/M$ ). Note that  $R \in [0, 1]$ , where  $R = 1$  indicates Student perfect learning (and  $R \geq 0$  because there no Students that predict more than half the Teacher labels incorrectly).

1785 **Derivation of the ST error ( $\epsilon(R)$ ) for the Linear Perceptron.** To derive Eqn. 90, define  
 1786 the data-dependent ST error (Eqn. 86) in terms of an  $\ell_2$  loss function.  
 1787 Write the data-averaged ST error as

$$E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) = \frac{1}{2} \sum_{\mu=1}^n (\mathbf{y}_\mu^S - \mathbf{y}_\mu^T)^\top (\mathbf{y}_\mu^S - \mathbf{y}_\mu^T) \quad (91)$$

1788 Define the  $n$  label vectors  $\mathbf{y}^S := [\mathbf{y}_{\mu=1}^S, \mathbf{y}_{\mu=2}^S, \dots, \mathbf{y}_{\mu=n}^S]$  and  $\mathbf{y}^T := [\mathbf{y}_{\mu=1}^T, \mathbf{y}_{\mu=2}^T, \dots, \mathbf{y}_{\mu=n}^T]$ . This lets us  
 1789 write the total Energy as

$$\begin{aligned} E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) &= \frac{1}{2} \text{Tr}[(\mathbf{y}^S - \mathbf{y}^T)^\top (\mathbf{y}^S - \mathbf{y}^T)] \\ &= \frac{1}{2} \text{Tr}[(\mathbf{y}^S)^\top \mathbf{y}^S - 2(\mathbf{y}^S)^\top \mathbf{y}^T + (\mathbf{y}^T)^\top \mathbf{y}^T] \\ &= n - \text{Tr}[(\mathbf{y}^S)^\top (\mathbf{y}^T)] \\ &= n - \text{Tr}[\eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n)], \end{aligned} \quad (92)$$

1790 where we define the *data-dependent Self-Overlap*:

$$\eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) := (\mathbf{y}^S)^\top (\mathbf{y}^T) \quad (93)$$

1791 The expression  $\eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n)$  is analogous to the ST overlap  $R$ , but before the data has been  
 1792 integrated out. It is convenient to work directly with the Self-Overlap  $\eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n)$  because it  
 1793 will appear later in Eqn. 107 (in Section 5), when formulating the matrix-generalized overlap  
 1794 operator  $\mathbf{R}$ .

1795 In defining  $\eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n)$ , we replace the individual labels  $(\mathbf{y}_\mu^S, \mathbf{y}_\mu^T)$  with the Energy functions  
 1796  $E_{NN}^{\text{out}}$  that generate them, giving an expression in terms of the weights  $(\mathbf{s}, \mathbf{t})$  and the Gaussian  
 1797 data variables  $(\boldsymbol{\xi})$ . We will then integrate out the data variables, leaving an expression just in  
 1798 terms of the weights. Using the  $E_{NN}^{\text{out}}$  Energy generating or output function (Eqn. 1, 4.3.1, 77),  
 1799 we can write the labels as

$$\mathbf{y}_\mu^S = \mathbf{s}^\top \boldsymbol{\xi}_\mu, \quad \mathbf{y}_\mu^T = \mathbf{t}^\top \boldsymbol{\xi}_\mu. \quad (94)$$

1800 This now gives the data-dependent Self-Overlap explicitly as

$$\eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) = \sum_{\mu=1}^n (\mathbf{s}^\top \boldsymbol{\xi}_\mu)^\top (\mathbf{t}^\top \boldsymbol{\xi}_\mu) = \sum_{\mu=1}^n \boldsymbol{\xi}_\mu^\top (\mathbf{s}^\top \mathbf{t}) \boldsymbol{\xi}_\mu \quad (95)$$

1801 After integrating over the data, we have the *data-independent Self-Overlap*,  $\eta(\mathbf{s}, \mathbf{t})$ :

$$\begin{aligned} \eta(\mathbf{s}, \mathbf{t}) &:= \langle \eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \rangle_{\bar{\boldsymbol{\xi}^n}} = \frac{1}{n} \int d\mu(\boldsymbol{\xi}^n) \eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \\ &= \frac{1}{n} \int d\mu(\boldsymbol{\xi}^n) \sum_{\mu=1}^n \boldsymbol{\xi}_\mu^\top \mathbf{s}^\top \mathbf{t} \boldsymbol{\xi}_\mu \\ &= \frac{1}{n} \int d\mu(\boldsymbol{\xi}^n) \sum_{\mu=1}^n \boldsymbol{\xi}_\mu^\top R \boldsymbol{\xi}_\mu \\ &= R \frac{1}{n} \sum_{\mu=1}^n \int d\mu(\boldsymbol{\xi}_\mu) \boldsymbol{\xi}_\mu^\top \boldsymbol{\xi}_\mu \\ &= R. \end{aligned} \quad (96)$$

1802 where the third equality holds because  $R$  is a scalar constant, and the fourth holds because  
1803 the elements of  $\boldsymbol{\xi}$  are i.i.d. and normalized to unit variance. (See Section A.2.1) .

1804 We can now obtain the Annealed Error Potential  $\epsilon(R)$  for the data-averaged ST test error  
1805 (see Eqn. 30), as in Eqn. 90,

$$\epsilon(R) = \langle E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \rangle_{\bar{\boldsymbol{\xi}^n}} = 1 - R. \quad (97)$$

1806 In traditional **StatMech** (e.g., [8]), one is interested in how the *Total Generalization Error*  
1807  $\mathcal{E}_{gen}(R)$  depends on  $R$ . With these simple error functions, Eqn. 88 reduces to a function over  $R$ ,  
1808 and the Average ST Generalization Error  $\mathcal{E}_{gen}^{ST}(R)$  is then obtained by taking a *Thermal Average*  
1809 over the Students

$$\bar{\mathcal{E}}_{gen}^{ST}(R) = \langle \epsilon(R) \rangle_{\mathbf{s}}^\beta = \left\langle 1 - \langle \eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \rangle_{\bar{\boldsymbol{\xi}^n}} \right\rangle_{\mathbf{s}}^\beta = \langle 1 - \eta(\mathbf{s}, \mathbf{t}) \rangle_{\mathbf{s}}^\beta = \langle 1 - \mathbf{s}^\top \mathbf{t} \rangle_{\mathbf{s}}^\beta = \langle (1 - R) \rangle_{\mathbf{s}}^\beta, \quad (98)$$

1810 where  $\langle \dots \rangle_{\mathbf{s}}^\beta$  is a Thermal Average over the Student weight vector  $\mathbf{s}$ . Recall that even at high-T,  
1811 this restricts the Students to ones trained with a similar amount of regularization as the Teacher  
1812 (i.e. the measure  $d\mu(\mathbf{s}) = d\mathbf{s}$  is independent of  $\beta$ ).

1813 The average Quality for the ST Perceptron,  $\bar{\mathcal{Q}}^{ST}$ , is just the Average Generalization Accuracy,  
1814 so we can write

$$\bar{\mathcal{Q}}^{ST} := 1 - \bar{\mathcal{E}}_{gen}^{ST}(R) = \langle 1 - \epsilon(R) \rangle_{\mathbf{s}}^\beta = \left\langle \langle \eta(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \rangle_{\bar{\boldsymbol{\xi}^n}} \right\rangle_{\mathbf{s}}^\beta = \langle \eta(\mathbf{s}, \mathbf{t}) \rangle_{\mathbf{s}}^\beta = \langle \mathbf{s}^\top \mathbf{t} \rangle_{\mathbf{s}}^\beta = \langle R \rangle_{\mathbf{s}}^\beta. \quad (99)$$

1815 Eqn. 99 is the starting point for deriving a **SemiEmpirical** theory for the **WeightWatcher** quality  
1816 metrics (**Alpha**, **AlphaHat**); see Section 5.1. To generalize this expression, we will start with the  
1817 Self-Overlap  $\eta(\mathbf{S}, \mathbf{T}, \boldsymbol{\xi}^n)$  for a Multi-Layer Perceptron (MLP3) in Section 5.

1818 Before doing this, however, we note that we can obtain this expression for  $\bar{\mathcal{E}}_{gen}^{ST}$  by defining  
1819 the Annealed Hamiltonian  $H_{hT}^{an}(R)$ , at high-Temperature, as in Section 4.2, Eqn. 49. Indeed, it  
1820 is really  $H_{hT}^{an}(R) = \epsilon(R)$  that we must generalize to the matrix case in the next section, which we  
1821 do (using a technique similar to a Replica calculation, but still in the AA).

Quantity	Traditional SMOG	Linear Perceptron in Traditional SMOG	Matrix Generalization for SETOL
Total (Idealized) Data Error	$E_{\mathcal{L}}^n(\mathbf{w}, \boldsymbol{\xi}^n)$ (31)	$E_{\mathcal{L}}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n)$ (91)	$E_{\ell_2}^n(\mathbf{S}, \mathbf{T}, \boldsymbol{\xi}^n)$ (102)
Annealed Hamiltonian (Data-Averaged Error)	$H_{hT}^{an} = \epsilon(\mathbf{w})$ (30) (AA, at high-T)	$H_{hT}^{an}(R) = \epsilon(\mathbf{s}, \mathbf{t}) = 1 - R$ (97) (and at Large- $\mathcal{N}$ )	$H_{hT}^{an}(\mathbf{R}) = N(\mathbf{I}_M - \mathbf{R})$ (206) (only for a layer)
Self-Overlap	$\eta(\mathbf{w}) = 1 - \epsilon(\mathbf{w})$ (32)	$\eta(\mathbf{s}, \mathbf{t}) = \mathbf{s}^\top \mathbf{t}$ (96)	$\eta(\mathbf{S}, \mathbf{T}) = \frac{1}{N} \mathbf{S}^\top \mathbf{T}$ (107)
Model Quality in terms of Layer Quality	$\bar{\mathcal{Q}} := 1 - \bar{\mathcal{E}}_{gen}$	$\bar{\mathcal{Q}}^{ST} := 1 - \bar{\mathcal{E}}_{gen}^{ST}$ (60)	$\bar{\mathcal{Q}}^{NN} := 1 - \bar{\mathcal{E}}_{gen}^{NN}$ (60) $\bar{\mathcal{Q}}^{NN} := \prod_L \bar{\mathcal{Q}}_L^{NN}$

Table 7: Summary of key quantities compared across traditional SMOG models, the Student-Teacher (ST) Linear Perceptron in the Annealed Approximation (AA) and at high-Temperature (high-T) and at Large- $\mathcal{N}$  in  $n$ , and the matrix-generalized forms as the starting point to frame SETOL. The total ST Error of Energy,  $E_{\mathcal{L}}^n$ , represents the difference (squared) between the model and its labels for the ST model between the Student and Teacher predictions. The Annealed Hamiltonian is the Energy function for this Error after it is averaged over the model for the training data (an  $n$ -dimensional i.i.d. idealized Gaussian dataset,  $\boldsymbol{\xi}^n$ ). In the AA, the Annealed Hamiltonian is equal to the Annealed Error Potential. For the ST model, this is one minus the average overlap,  $H_{hT}^{an}(R) = (1 - R)$ ; for the SETOL, this is the ( $M$ -dimensional) identity minus the overlap operator/matrix,  $H_{hT}^{an}(\mathbf{R}) = N(\mathbf{I}_M - \mathbf{R})$ . The Self-Overlap  $\eta(\dots)$  is used to describe the Accuracy (as opposed to the Error) for both the ST model and its matrix-generalized form. Finally, the different forms of the Quality are defined. Generally speaking, the Quality  $\bar{\mathcal{Q}}$  is an approximation to some measure of 1 minus the Average Generalization Error,  $\bar{\mathcal{Q}} := 1 - \bar{\mathcal{E}}_{gen}$  (in the AA, at high-T, at Large- $\mathcal{N}$ , and with whatever else approximations are applied). For the ST model, having just 1 layer, the Model Quality and the Layer Quality are the same, and denoted  $\bar{\mathcal{Q}}^{ST}$ . For SETOL, the Model Quality  $\bar{\mathcal{Q}}^{NN}$  is a product of individual Layer Qualities  $\bar{\mathcal{Q}}_L^{NN}$ . (Note that the final SETOL Layer Quality  $\bar{\mathcal{Q}}$  is defined in terms of the Layer Quality-Squared  $\bar{\mathcal{Q}}^2$ , and the starting point for this is expressed with the Layer Quality-Squared Hamiltonian  $\mathbf{H}_{\bar{\mathcal{Q}}^2} = \mathbf{R}^\top \mathbf{R}$ ).

**Final Remarks.** Additional results are provided in Appendix A.2. In particular, In Appendix A.2.1, we use the ideas from this section and the previous one to derive the full non-linear vector form of the Annealed Hamiltonian  $H^{an}(\mathbf{w})$  (Eqn. 43) for the Linear Perceptron, in the AA. Then, in Appendix A.2.1, we derive the matrix generalization  $H^{an}(R) \rightarrow H^{an}(\mathbf{R})$  of these quantities using a Large- $\mathcal{N}$  in  $n$  expansion (as opposed to a full replica calculation). This derivation explains how to obtain the implicit  $1/M$  normalization for the weight matrices  $\mathbf{W}$  that is necessary for the final results in Section 5. (Notice this is similar to the implicit normalization  $1/m$  on the ST vectors) Then, taking the case  $N = 1$ , we can recover the original result for  $H^{an}(R)$ . We can then express the Annealed Hamiltonian at High-T, i.e.,  $H_{hT}^{an}(R) = \epsilon(R)$  (Eqn. 49). This shows that our new derivation is consistent with the full and the High-T results for classic ST Perceptron model, for a Linear Perceptron in the AA. [8]

## 5 Semi-Empirical Theory of the HTSR Phenomenology

In this section, we present the main technical elements of our Semi-Empirical Theory of Deep Learning (SETOL). Our goal is to explain and, where possible, derive the HTSR PL metrics  $\alpha$  and  $\hat{\alpha}$  from first principles, and, in doing so, also present the **ERG** condition and newly proposed **WeightWatcher DetX** metric. To do this, we introduce a Matrix Generalization of the Student-Teacher model for a Linear Perceptron (See Section 4.3.2), adapted here for a (3-layer) Multi-Layer Perceptron (MLP3). We seek a theory for the Layer Quality  $\bar{Q} = \bar{Q}_L^{NN}$  of a NN, where this Layer Quality now corresponds to the (approximate) contribution each layer makes to the total generalization accuracy, or total Quality  $\bar{Q}^{NN}$ . For technical reasons, we actually seek a formal expression(s) for the Layer Quality-Squared,  $\bar{Q}^2 \approx (\bar{Q}_L^{NN})^2$ . We say that the SETOL is Semi-Empirical because the final result  $\bar{Q}^2$  is expressed directly in terms of the empirically observable spectral properties of the Teacher layer weight matrix  $\mathbf{T} = \mathbf{W}$ .

**5.1 Matrix Generalization of the ST Model.** Section 5.1 generalizes classical StatMech vector-based ST model of Section 4.3 to obtain a Layer Quality for a single layer in an NN. It starts by first formulating the learning problem for the NN generalization accuracy or quality,  $\bar{Q}^{NN}$ , of a 3-layer MLP (MLP3). We then replace vectors with  $N \times M$  matrices  $\mathbf{s}, \mathbf{t} \rightarrow \mathbf{S}, \mathbf{T}$ , and obtain an expression for the NN Self-Overlap  $\eta(\mathbf{S}, \mathbf{T}, \xi^n)$ , which then gives a matrix-generalized overlap operator  $\mathbf{R} := \langle \eta(\mathbf{S}, \mathbf{T}, \xi^n) \rangle_{\xi^n} = \frac{1}{N} \mathbf{S}^\top \mathbf{T}$ . This can be related to a single-layer matrix-generalization of the ST Annealed Hamiltonian, presented in Appendix A.2,  $H_{hT}^{an}(\mathbf{R}) := N(\mathbf{I}_M - \mathbf{R})$ , where, importantly, the scalar overlap  $R$  is now a matrix  $\mathbf{R}$  of  $M \times M$  adjustable parameters. Importantly, being empirical quantities, the weight matrices are implicitly normalized by  $1/n$ , and, like the ST vectors, also implicitly normalized by  $1/M$ . (See Appendix A.2.2).

**5.2 The Layer Quality-Squared  $\bar{Q}^2$ .** Section 5.2 presents the expression for NN Layer Quality-Squared  $\bar{Q}^2$ . Following the ST analogy, we define a Thermal Average over possible Student weight matrices  $\mathbf{S}$  for the matrix overlap, giving  $\bar{Q}_L^{NN} := \langle H_{hT}^{an} \rangle_{\mathbf{S}}^\beta = \langle \mathbf{R} \rangle_{\mathbf{S}}^\beta$ . For technical reasons, however, we actually seek the (approximate) Layer Quality-Squared,  $\bar{Q}^2 \approx (\bar{Q}_L^{NN})^2$ , defined as  $\bar{Q}^2 := \langle \mathbf{R}^\top \mathbf{R} \rangle_{\mathbf{S}}^\beta$ . To evaluate  $\bar{Q}^2$ , rather than sampling all random Student matrices  $\mathbf{S}$  directly, we switch measures to the (Outer) Student Correlation matrices<sup>35</sup>  $\mathbf{A}_N = \frac{1}{N} \mathbf{S} \mathbf{S}^\top$  along with their Inner counterparts  $\mathbf{A}_M = \frac{1}{N} \mathbf{S}^\top \mathbf{S}$ . Importantly, we argue that the measures  $d\mu(\mathbf{A}_M) \leftrightarrow d\mu(\mathbf{A}_N)$ , can be interchanged for our purposes, making them effectively equivalent. This reparameterization leads us to an integral of the HCIZ type (as in Eqn. 73) which, as shown by Tanaka [83, 84], is expressed in terms of the R-transform  $R_{\mathbf{A}_M}(z)$ , defined for the tail of the limiting form of the ESD of  $\mathbf{A}_M$ ,  $\rho_{\mathbf{A}_M}^\infty(\lambda)$ .

Then, we introduce the Effective Correlation Space (ECS), and two key approximations, the Independent Fluctuation Approximation (IFA) and the Exact Renormalization Group (ERG) Condition. We impose the IFA (described below) because it is necessary for the final result. The ERG condition states that the determinant of the (effective) Student correlation matrix is unity,  $\det(\tilde{\mathbf{A}}) = 1$ . Critically, this condition can be tested empirically by assuming the (effective) Teacher correlation matrix also follows the testable ERG condition,  $\det(\tilde{\mathbf{X}}) = 1$ . **The empirically testable ERG condition is a key result of this work.**

**5.3 The Wide Layer Large- $\mathcal{N}$  limit in  $N$ .** Section 5.3 presents the core result, (as in Eqn. 15), closed-form or semi-analytic expression(s) for the Layer Quality-Squared  $\bar{Q}^2$

<sup>35</sup>We adopt the convention “Inner” for smaller,  $M \times M$  full rank Student correlation matrices, and “Outer” for larger,  $N \times N$  rank-deficient Student Correlation matrices. Note that both are scaled as  $1/N$ , meaning that their nonzero eigenvalues are the same.

formed in the Wide Layer Large- $\mathcal{N}$  limit in  $N$ . Restricted to the ECS, and under the ERG condition and the IFA, our HCIZ integral for  $\bar{Q}^2$  becomes tractable at large- $N$ , giving an expression that can be parameterized in terms of  $\tilde{M}$  eigenvalues  $\tilde{\lambda}$  of the Teacher correlation matrix restricted to the ECS  $\tilde{\mathbf{X}}$ . In doing this, the  $\tilde{M}$  Teacher eigenvalues are treated as experimental observables, and become the effective Semi-Empirical parameters (i.e.,  $\alpha$ ,  $\lambda_{max}$ ) of the SETOL approach.

**5.4 Selecting the Heavy-Tailed R-transform.** Section 5.4 presents several models of different R-transforms. Evaluating  $\bar{Q}^2$  requires evaluating selecting an R-transform  $R(z)$  for the Teacher Empirical Spectral Density (ESD), and also ensure that it is analytic and single-valued on the domain of interest—the ECS and/or tail of the ESD. We examine four possible models for  $R(z)$ : (i) the *Bulk+Spikes* (BS), (ii) the *Free Cauchy* (FC) model, (iii) the *Inverse Marchenko-Pastur* (IMP) model, and (iv) the Levy-Wigner (LW) model. First, as a trivial case, the tail of ESD can be treated as a collection of spikes, and the ESD is simply a sum of Dirac delta functions; in this case,  $\bar{Q}^2$  becomes a “Tail Norm”, the Frobenius Norm of the PL tail. When the layer is Ideal, i.e.,  $\alpha \sim 2$  and  $\det(\tilde{\mathbf{X}}) \sim 1$ , one can use *Free Cauchy* (FC) model. and the resulting Layer Quality  $\bar{Q}$  is approximately the Spectral Norm  $\lambda_{max}$ . Since  $\lambda_{max}$  increases with decreasing  $\alpha$ , the FC model yields the HTSR Alpha metric. One can also use *Inverse Marchenko-Pastur* (IMP) model. Being a model for the full Teacher ESD (not just the tail) the IMP R-transform contains a *branch cut* in the complex plane which aligns with the start of the ECS Power Law tail. Finally, Using the Levy-Wigner (LW) model, one can model cases where  $\alpha \leq 2$  and derive the HTSR AlphaHat metric.

These core elements form a bridge between well-established empirical properties of large-scale NNs and a tractable ST-based theory. In the subsequent sections, we formalize the key steps: (i) setting up the matrix-based ST problem, (ii) defining our HCIZ integrals over restricted correlation matrices (ECS), and (iii) analyzing the resulting *Layer Quality* (or *Quality-Squared*) expressions in the Large- $\mathcal{N}$  limit in  $N$ .

## 5.1 Multi-Layer Setup: MLP3

In this section, we describe the matrix generalization of the ST model of the Linear Perceptron; and, in particular, a matrix-generalized version of the key quantities we derived in Section 4.3.2.

**A simple model.** Consider a simple NN with three layers (two hidden and an output), i.e., a three-layer Multi-Layer Perceptron, denoted as the *MLP3* model. (This is a *very* simple model of a modern NN with hundreds of layers and complex internal structure.)

Ignoring the bias terms, *Without Loss of Generality*, (WLOG), the NN outputs  $E_{1\mu}, E_{2\mu}, E_{3\mu}$  for each layer, as defined in Eqn. 1, are given by:

$$\begin{aligned} \mathbf{E}_{1\mu}^{out} &:= \frac{1}{\sqrt{N_1}} h(\mathbf{W}_1^\top \boldsymbol{\xi}_\mu), \\ \mathbf{E}_{2\mu}^{out} &:= \frac{1}{\sqrt{N_2}} h(\mathbf{W}_2^\top \mathbf{E}_{1\mu}^{out}), \\ y_\mu &:= \mathbf{E}_{3\mu}^{out} = \frac{1}{\sqrt{N_3}} h(\mathbf{W}_3^\top \mathbf{E}_{2\mu}^{out}), \end{aligned} \tag{100}$$

where  $\mathbf{E}_{\# \mu}^{out}$  denotes a vector of energies or NN outputs for that layer, and  $h$  is a general function or functional, denoting either a non-linear activation or a more complex layer structure, such as

1912 a CNN or an RNN. Note that for binary classification,  $\mathbf{E}_{3\mu}^{out} = 1| - 1$  is just a binary number. We  
 1913 can consider  $h(\cdot)$  to be an (unspecified) activation function, but here we simply take  $h(x) = x$ .

1914 As in Eqn. 91, let us specify the ST error, or total Energy, specifically in terms of the  $\ell_2$  or  
 1915 MSE loss:

$$E_{\ell_2}^n(\mathbf{S}, \mathbf{T}, \boldsymbol{\xi}^n) = \frac{1}{2} \sum_{\mu=1}^n (y_{\mu}^S - y_{\mu}^T)^2. \quad (101)$$

1916 We now develop the matrix generalized form of the self-overlap  $\eta$ :

### 1917 5.1.1 Data-Dependent Multi-Layer ST Self-Overlap ( $\eta(\mathbf{S}, \mathbf{T})$ )

1918 Following the same approach in Section 4.3.2, it is convenient to rewrite the total Energy  $E_{\mathcal{L}}^n$  in  
 1919 Eqn. 101 as:

$$E_{\ell_2}^n(\mathbf{S}, \mathbf{T}, \boldsymbol{\xi}^n) := \frac{1}{2} \text{Tr}[(\mathbf{y}^S - \mathbf{y}^T)^\top (\mathbf{y}^S - \mathbf{y}^T)] = n - \text{Tr}[(\mathbf{y}^S)^\top \mathbf{y}^T] = n - \eta([\mathbf{S}_l, \mathbf{T}_l], \boldsymbol{\xi}^n) \quad (102)$$

1920 where the Self-Overlap  $\eta([\mathbf{S}_l, \mathbf{T}_l], \boldsymbol{\xi}^n)$  is of the same form as the (vector) Linear Perceptron (in  
 1921 Eqn. 91). Note that  $\eta([\mathbf{S}_l, \mathbf{T}_l], \boldsymbol{\xi}^n)$  depends on the (idealized) data  $\boldsymbol{\xi}^n$  because we have not  
 1922 evaluated the expected value  $\langle \dots \rangle_{\boldsymbol{\xi}^n}$  yet.

1923 Using the general expression from Eqn. 100 for the action of the NN on the input data  $\boldsymbol{\xi}$ , we  
 1924 can write the formal expression of the ST error for the simple MLP3 model as:

$$\begin{aligned} \langle \eta([\mathbf{S}_l, \mathbf{T}_l], \boldsymbol{\xi}^n) \rangle_{\boldsymbol{\xi}^n} &= \langle \eta(\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, \mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3, \boldsymbol{\xi}^n) \rangle_{\boldsymbol{\xi}^n} \\ &:= \frac{1}{n} \text{Tr} \left[ \left\{ \frac{1}{\sqrt{N_3}} h \left( \mathbf{S}_3^\top \frac{1}{\sqrt{N_2}} h \left( \mathbf{S}_2^\top \frac{1}{\sqrt{N_1}} h \left( \mathbf{S}_1^\top \boldsymbol{\xi}^n \right) \right) \right) \right\}^\top \right. \\ &\quad \left. \times \frac{1}{\sqrt{N_3}} h \left( \mathbf{T}_3^\top \frac{1}{\sqrt{N_2}} h \left( \mathbf{T}_2^\top \frac{1}{\sqrt{N_1}} h \left( \mathbf{T}_1^\top \boldsymbol{\xi}^n \right) \right) \right) \right] \end{aligned} \quad (103)$$

1925 So far, we have not used any particular assumption on the form of the NN or the data, other  
 1926 than that the layer structure used to write the explicit expression for the form eventually needed,  
 1927  $\eta(\mathbf{S}, \mathbf{T})$ , a single layer Self-Overlap. As a next step, we show which assumptions are needed in  
 1928 order to reformulate the setup as an effectively a single layer linear model for a NN.

### 1929 5.1.2 A Single Layer Matrix Model

1930 Following others in the literature [110], and for simplicity, one can restrict to the simplifying case  
 1931 that the function  $h(x)$  is the identity function. To evaluate Eqn. 103, there are three possibilities.  
 1932 First, we can multiply all the matrices together, and treat a multi-layer NN effectively as a single  
 1933 layer. Under this assumption, Eqn. 103 simplifies to

$$\langle \eta([\mathbf{S}_l, \mathbf{T}_l], \boldsymbol{\xi}^n) \rangle_{\boldsymbol{\xi}^n} = \frac{1}{n} \frac{1}{N_3 N_2 N_1} \text{Tr}[(\boldsymbol{\xi}^n)^\top \mathbf{S}_1 \mathbf{S}_2 \mathbf{S}_3 \mathbf{T}_3^\top \mathbf{T}_2^\top \mathbf{T}_1^\top (\boldsymbol{\xi}^n)]. \quad (104)$$

1934 While this is possible, it would not lead to layer-by-layer insights (as HTSR-based approaches do).  
 1935 Second, we could attempt to expand Eqn. 104 into inter- and intra-layer terms, which we could  
 1936 readily do if the  $S$  and  $T$  matrices were square and the same shape, and then apply Wick's  
 1937 theorem:

$$\eta([\mathbf{S}_l, \mathbf{T}_l]) \approx \frac{1}{n} \prod_{l=1}^L \frac{1}{N_l} \langle \eta(\mathbf{S}_l, \mathbf{T}_l, \boldsymbol{\xi}^n) \rangle_{\boldsymbol{\xi}^n} = \frac{1}{n} \prod_{l=1}^L \frac{1}{N_l} \text{Tr}[(\boldsymbol{\xi}^n)^\top \mathbf{S}_l^\top \mathbf{T}_l (\boldsymbol{\xi}^n)] + \text{intra-layer cross terms.} \quad (105)$$



However, these matrices are not square, and we don't know how to express the intra-layer cross terms. Finally, we can simply assume that the individual layers are statistically independent, in which case we can treat each layer independently. By ignoring the intra-layer cross-terms, let us write the single-layer self-overlap  $\eta(\mathbf{S}_l, \mathbf{T}_l, \boldsymbol{\xi}^n)$  as:

$$\eta(\mathbf{S}_l, \mathbf{T}_l, \boldsymbol{\xi}^n) = \langle \eta(\mathbf{S}_l, \mathbf{T}_l, \boldsymbol{\xi}^n) \rangle_{\boldsymbol{\xi}^n} \rightarrow \frac{1}{n} \frac{1}{N} \text{Tr} [(\boldsymbol{\xi}^n)^\top \mathbf{S}_l^\top \mathbf{T}_l (\boldsymbol{\xi}^n)]. \quad (106)$$

This third approach is the one we will adopt. Moving forward, we will drop the layer subscript,  $l$ , and we will consider a SETOL as a single-layer theory.

### 5.1.3 The Matrix-Generalized ST Overlap ( $\eta(\mathbf{S}, \mathbf{T})$ ).

We can now relate the Self-Overlap for the NN layer  $\eta(\boldsymbol{\xi})_l$  in Eqn. 106 as a matrix-generalized form of the ST Annealed Error Potential  $\epsilon(R) = 1 - R$ . Since we can interpret the Trace as an expected value over the model data  $\boldsymbol{\xi}^n$ , this gives the desired

$$\eta(\mathbf{S}, \mathbf{T}) := \frac{1}{N} \text{Tr} [\mathbf{S}^\top \mathbf{T}] \quad (107)$$

We have dropped the  $1/n$  because (as noted above), the  $1/n$  will be implicit in the  $\mathbf{T}$  and  $\mathbf{S}$  matrices because they represent empirical observables. That is, the weights are the learned parameters, effectively averaged over the entire real-world training data set  $\mathbf{D}$ . This is the matrix generalized form of Eqn. 96.

## 5.2 Quality Metrics of an Individual Layer as an HCIZ Integral

In this subsection, we describe how to generalize the (Thermal) average over the Students  $\langle \dots \rangle_{\mathbf{S}}^\beta$  to an integral over random Student matrices,  $\langle \dots \rangle_{\mathbf{S}}^\beta$ , called an HCIZ integral.

### 5.2.1 A Generating Function Approach to Average Quality-Squared of a Layer

For our matrix generalization, we need to express the Layer Quality  $\bar{\mathcal{Q}}$  in terms of the data-averaged Self-Overlap in Eqn. 107 for a individual layer.

- **Student-Teacher Overlap  $\mathbf{R}$**  For the vector-based Perceptron ST model, the data-averaged Self-Overlap appears in the expression for the Layer Quality in Eqn. 99, and is just the average ST vector overlap  $R = \mathbf{s}^\top \mathbf{t}$ . We define

$$\mathbf{R} = \frac{1}{N} \mathbf{S}^\top \mathbf{T}. \quad (108)$$

The overlap matrix  $\mathbf{R}$  describes the average interactions between  $N$  interacting  $M$ -dimensional layer (i.e., feature) vectors. Also, notice that we have dropped  $1/n$  term. For the vector-based ST model, the ST Quality  $\bar{\mathcal{Q}}^{ST}$  in Eqn. 99 is expressed as the Thermal Average  $\bar{\mathcal{Q}}^{ST}(R) = \langle R \rangle_{\mathbf{S}}^\beta$ . We seek a similar formal expression for the individual matrix-generalized Layer Quality  $\bar{\mathcal{Q}}_L^{NN}$ , this time in terms of  $\mathbf{R}$  and a matrix-generalized Thermal Average.

- **Model and Layer Qualities  $\bar{\mathcal{Q}}^{NN}$ ,  $\bar{\mathcal{Q}}_L^{NN}$**  We define the Model Quality  $\bar{\mathcal{Q}}^{NN}$ , as explained in Subsection 2.3, Eqn. 7, to be a product of individual NN Layer Qualities  $\bar{\mathcal{Q}}_L^{NN}$ , and, as in Eqn. 60, approximates the total NN Average Generalization Accuracy  $(1 - \bar{\mathcal{E}}_{gen}^{NN})$ :

$$\bar{\mathcal{Q}}^{NN} := \prod_L \bar{\mathcal{Q}}_L^{NN} \approx 1 - \bar{\mathcal{E}}_{gen}^{NN} \quad (109)$$

The individual  $\bar{\mathcal{Q}}_L^{NN}$  expresses the contribution that layer makes to the approximate total NN Average Generalization Accuracy.

- **Layer Quality-Squared  $\bar{Q}^2$**  For technical convenience, however, rather than compute the NN Layer Quality  $\bar{Q}_L^{NN}$  directly, we will work with the *Average Layer Quality-Squared*, defined as

$$\bar{Q}^2 := \langle \mathbf{R}^\top \mathbf{R} \rangle_{\mathbf{S}}^\beta \quad (110)$$

where  $\langle \dots \rangle_{\mathbf{S}}^\beta$  is now a Thermal Average over Student weight matrices  $\mathbf{S}$ — an HCIZ integral. This choice means that the final Layer Quality  $\bar{Q}$  we use approximates what would be the matrix-generalized NN Layer Quality  $\bar{Q}_L^{NN}$  (above) as

$$\begin{aligned} \bar{Q} &:= \sqrt{\bar{Q}^2} = \sqrt{\langle \mathbf{R}^\top \mathbf{R} \rangle_{\mathbf{S}}^\beta} \\ &\approx \left\langle \sqrt{\mathbf{R}^\top \mathbf{R}} \right\rangle_{\mathbf{S}}^\beta \\ &\approx \langle \mathbf{R} \rangle_{\mathbf{S}}^\beta \\ &= \bar{Q}_L^{NN} \end{aligned} \quad (111)$$

- **Overlap Squared** The Overlap operator (squared)  $\text{Tr}[\mathbf{R}^\top \mathbf{R}]$  is defined in terms of Eqn. 116 such that we can

$$\bar{Q}^2 := \text{Tr}[\mathbf{R}^\top \mathbf{R}] = \frac{1}{N^2} \text{Tr}[\mathbf{T}^\top \mathbf{S} \mathbf{S}^\top \mathbf{T}] = \frac{1}{N} \text{Tr}[\mathbf{T}^\top \mathbf{A}_N \mathbf{T}]. \quad (112)$$

This choice, (as opposed to  $\text{Tr}[\mathbf{R} \mathbf{R}^\top]$ , which would correspond with Eqn. 115,) places  $\bar{Q}^2$  in the form of the HCIZ integral, as in Eqn. 73. See Appendix A.6 for a detailed discussion of why we define  $\bar{Q}^2$  using the *Outer* Student Correlation matrix  $\mathbf{A}_N$  (defined in Section 3, and Eqn. 116 below).

- **Generating Function** For the vector-based ST model, we could compute  $\bar{Q}^{ST}$  using a generating function,  $\beta \mathbf{\Gamma}_{\bar{Q}}^{ST}$ . For our matrix generalization, we compute  $\bar{Q}$  from a *Layer Quality-Squared Generating Function*  $\beta \mathbf{\Gamma}_{\bar{Q}^2}^{IZ}$ , given as

$$\beta \mathbf{\Gamma}_{\bar{Q}^2}^{IZ} := \frac{1}{N} \ln \int d\mu(\mathbf{S}) \exp[n\beta N \text{Tr}[\mathbf{R}^\top \mathbf{R}]]. \quad (113)$$

We normalize the  $\beta \mathbf{\Gamma}_{\bar{Q}^2}^{IZ}$  because we are going to take the Large- $\mathcal{N}$  limit in  $N$ , and we need to keep the Layer Quality finite. This allows us to implicitly fix the effective load of the layer,  $n/N$ , as  $\beta \mathbf{\Gamma}_{\bar{Q}^2}^{IZ}$  is also in the Thermodynamic limit and therefore at Large- $\mathcal{N}$  in  $n$ , although we do not explicitly set the layer (feature vector) load  $n/N$ . See Appendix A.3 for the derivation of Eqn. 113 (and recall the discussion in Section 4.2).

We cannot evaluate Eqn. 113 directly; but we will be able to evaluate it if we transform it into an HCIZ integral (as in Eqn. 73). To do this, however, requires a trick which will allow us to work with different forms of the Student  $\mathbf{A}$  (and Teacher  $\mathbf{X}$ ) Correlation matrices.

**From weight matrices to Correlation matrices.** To evaluate  $\bar{Q}^2$  in terms of derivatives of Eqn. 113, we need to introduce the change of measure:

$$d\mu(\mathbf{S}) \rightarrow d\mu(\mathbf{A}), \quad (114)$$

and then restrict  $d\mu(\mathbf{A})$  to resemble just the generalizing eigenvectors of the Teacher correlation matrix  $\mathbf{X}$ . We have two choices for the Student Correlation Matrix  $\mathbf{A}$ , call them  $\mathbf{A}_M$  (Inner) and  $\mathbf{A}_N$  (Outer), defined as:

$$(\text{Inner}) \quad \mathbf{A}_M := \frac{1}{N} \mathbf{S}^\top \mathbf{S} \quad (\text{which is } M \times M) \quad (115)$$

$$(\text{Outer}) \quad \mathbf{A}_N := \frac{1}{N} \mathbf{S} \mathbf{S}^\top \quad (\text{which is } N \times N). \quad (116)$$

Note that  $\frac{1}{N}$  is the correct scaling on each of these. Eqn. 115 is consistent with our definition of the layer Correlation Matrix, and we use it as the starting point below to derive the Volume-Preserving ERG condition (Appendix A.4). Eqn. 116 is consistent with Tanaka, which requires  $\mathbf{A}$  be  $N \times N$ , but we still need a *Duality of Measures* to rederive this (Appendix A.6) [83, 84].

**Duality of measures.** For either form of  $\mathbf{A}$ , the measure  $d\mu(\mathbf{A})$  is the same because we will restrict the measures to the ECS space of non-zero eigenvalues ( $\lambda_i \gg 0$ ). We note that  $\mathbf{A}_M$  and  $\mathbf{A}_N$  have the same eigenvalues  $\lambda_i$ , or ESD, up to the additional zero eigenvalues ( $\lambda_i = 0$ ) in the null space of  $\mathbf{A}_N$ . Consequently, both forms of  $\mathbf{A}$  have the same non-zero part of the ESD ( $\rho(\lambda) \gg 0$ ), and the same Trace ( $\text{Tr}[\mathbf{A}_M] = \text{Tr}[\mathbf{A}_N]$ ). In the large- $N$  approximation, the ESD of (either form of)  $\mathbf{A}$ ,  $\rho_{\mathbf{A}}^\infty(\lambda)$ , becomes continuous (and bounded), but remains zero in the null space. (Notice that following the physics approach, in the limit,  $N$  remains finite but we nevertheless assume a continuous spectrum) Consequently, when integrating over the eigenvalues  $\lambda$ , one can interchange  $\mathbf{A}_M$  with  $\mathbf{A}_N$ , such that

$$\int d\mu(\mathbf{A}) [\dots] \leftrightarrow \int d\lambda [\dots] \rho_{\mathbf{A}_M}^\infty(\lambda) \leftrightarrow \int d\lambda [\dots] \rho_{\mathbf{A}_N}^\infty(\lambda) \quad (117)$$

This equivalence will be essential both to derive the ERG condition (Section A.4), and to (re)derive the core result by Tanaka (Section A.6). Additionally, and WLOG, we may occasionally denote the Student Correlation matrix as  $\tilde{\mathbf{A}}$  instead of explicitly using  $\mathbf{A}_M$  and  $\mathbf{A}_N$ .

### 5.2.2 Evaluating the Average Quality (Squared) Generating Function

We can write the generating function  $\beta \Gamma_{Q^2}^{IZ}$  in Eqn. 113 in terms of  $\mathbf{A}_N$ , giving, as in Eqn. 12,

$$\beta \Gamma_{Q^2}^{IZ} = \frac{1}{N} \ln \int d\mu(\mathbf{S}) e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} \quad (118)$$

To recast Eqn. 118 as an HCIZ integral, as in Eqn. 73, we must perform a change of measure, from  $N \times M$  Student weight matrices  $\mathbf{S}$  to  $N \times N$  Outer Student Correlation matrices  $\mathbf{A}_N$ , as in Eqn. 114.

When we perform the change of measure on Eqn. 118, we obtain the following expression:

$$\begin{aligned} \beta \Gamma_{Q^2}^{IZ} &\approx \frac{1}{N} \ln \int d\mu(\mathbf{A}) e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\mathbf{A}_M))} \\ &= \frac{1}{N} \ln \left\langle e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\mathbf{A}_M))} \right\rangle_{\mathbf{A}} \end{aligned} \quad (119)$$

where the latter expresses the former in Bra-Ket notation. Since the measures of  $\mathbf{A}_M$  and  $\mathbf{A}_N$  are equivalent, this evaluates to the same quantity regardless of which is used. This expression is derived in Appendix A.4 (see Eqn. 249): it contains the original overlap term that depends  $\mathbf{A}_N$  as well as a new term from the transformation that depends on  $\det(\mathbf{A}_M)$  that is not yet defined.

### 5.2.3 The Effective Correlation Space (ECS)

Currently, Eqn. 119 is a “formal” expression, and we have not identified and/or justified its realm of applicability. Fortunately, we have empirical evidence to suggest that this can be made “physically” meaningful, by “restricting” the integral to the tail of the Empirical Spectral Density (ESD). Since the ESD is an empirical object, this is where the theory becomes Semi-Empirical.

Prior work on HTSR theory indicates that during training the generalizing parts of a layer weight matrix concentrate into  $\rho_{tail}^{emp}(\lambda)$ , the tail of the ESD, as the ESD becomes more Power Law (PL), and layer PL exponent  $\alpha \rightarrow 2+$  (from above) [63, 64, 25, 26, 28]. This suggests the integral in Eqn. 9 should instead average over a low rank subspace spanned *only by* the generalizing eigen-components of the Inner Correlation matrix,  $\mathbf{A}_M = \frac{1}{N} \mathbf{S}^\top \mathbf{S}$  (or equivalently, the Outer Correlation matrix  $\mathbf{A}_N$ ). **We call this subspace the Effective Correlation Space (ECS).**

Let  $\tilde{\mathbf{A}}$  be the matrix spanned by the largest  $\tilde{M}$  eigen-components  $\mathbf{A}$  in either form,  $\mathbf{A}_M$  (Inner) or  $\mathbf{A}_N$  (Outer), and using physics BraKet notation, giving

$$\tilde{\mathbf{A}} := \mathbf{P}_{ecs} \mathbf{A}, \quad \mathbf{P}_{ecs} := \sum_{i=1}^{\tilde{M}} |\tilde{\lambda}_i\rangle \langle \tilde{\lambda}_i| \quad (120)$$

where  $\mathbf{P}_{ecs}$  is the projection operator onto the subspace spanned by the eigenvector  $|\tilde{\lambda}_i\rangle$  associated with the eigenvalue  $\tilde{\lambda}_i$  of  $\mathbf{A}_M$  or, equivalently,  $\mathbf{A}_N$ . We denote the corresponding projected Student correlation matrices with a tilde, as follows:

$$\begin{aligned} \mathbf{A}_M &\rightarrow \tilde{\mathbf{A}}_M \text{ such that } d\mu(\mathbf{A}_M) \rightarrow d\mu(\tilde{\mathbf{A}}_M) \\ \mathbf{A}_N &\rightarrow \tilde{\mathbf{A}}_N \text{ such that } d\mu(\mathbf{A}_N) \rightarrow d\mu(\tilde{\mathbf{A}}_N) \end{aligned} \quad (121)$$

where now the matrices  $\tilde{\mathbf{A}}_M$  and  $\tilde{\mathbf{A}}_N$  are restricted to the ECS, and the measure  $d\mu(\tilde{\mathbf{A}}_M)$  is similarly restricted. We denote the eigenvalue  $\lambda$  with the tilde,  $\tilde{\lambda}$ , when we want to emphasize it is in the ECS—but may drop the tilde if it is clear from the context. See Appendix A.4 for more..

When an ESD is *Fat-Tailed* the ECS is at least as large if not larger than the PL tail of the ESD. For an ESD with  $\alpha \geq 2$ , the generalizing eigen-components, i.e.  $|\lambda_i\rangle$ , will mostly concentrate into the tail of the ESD, but some will remain in the bulk, so the ECS will be larger than the tail. In this case that  $\tilde{M} \geq M^{tail}$ , and  $\rho_{ECS}(\lambda) \supseteq \rho_{tail}(\lambda)$ , as depicted in Figure 5.2.4. When  $\alpha = 2$ , the layer is Ideal (as in Section 3.1), in that all of the generalizing eigen-components to have now concentrated completely into the tail, so that  $\tilde{M} = M^{tail}$ , and  $\rho_{ECS}(\lambda) = \rho_{tail}(\lambda)$ . (When  $\alpha < 2$ , this suggests that the layer is overfit, and the layer may have a Correlation Trap and/or frequently also has many near-zero eigenvalues.)

This leads to the following Model Selection Rule (MSR) for the ECS:

When transforming the measure  $d\mu(\mathbf{S}) \rightarrow d\mu(\tilde{\mathbf{A}})$ , we invoke an eigenvalue cutoff rule that prescribes how to replace  $\mathbf{A}$  with a low-rank effective matrix  $\mathbf{A} \rightarrow \tilde{\mathbf{A}}$ , where the cutoff  $\tilde{\lambda} \geq \tilde{\lambda}_{min}$  is chosen so that the ECS at least contains the PL tail and, importantly, such that  $\det(\mathbf{A}) = \det(\mathbf{A}_M) = \det(\mathbf{A}_N)$  is well defined.

Formally, this means that when we evaluate the Quality (squared)  $\bar{Q}^2$ , Generating Function  $\beta \Gamma_{\bar{Q}^2}^{IZ}$  or other relevant averages, we restrict the measure (i.e., integral or sum) to the eigencomponents in the tail of the ESD of  $\mathbf{A}$  (or  $\mathbf{X}$ , when appropriate) starting with  $\tilde{\lambda}_{min}$ . To our knowledge, this proposed MSR is completely novel.

Restricted to the ECS, we now replace Eqn. 119 with:

$$\begin{aligned}\beta\Gamma_{\tilde{\mathbf{Q}}^2}^{IZ} &= \frac{1}{N} \ln \int d\mu(\tilde{\mathbf{A}}) e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \tilde{\mathbf{A}}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\tilde{\mathbf{A}}_M))} \\ &= \frac{1}{N} \ln \left\langle e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \tilde{\mathbf{A}}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\tilde{\mathbf{A}}_M))} \right\rangle_{\tilde{\mathbf{A}}}\end{aligned}\quad (122)$$

where we have used the formal Duality of Measures,  $d\mu(\tilde{\mathbf{A}}) = d\mu(\tilde{\mathbf{A}}_M) = d\mu(\tilde{\mathbf{A}}_N)$ .<sup>36</sup>

#### 5.2.4 Two Simplifying Assumptions: the IFA and ERG Condition

It now remains how to define the cutoff for the ECS space. To accomplish this, we make the following assumptions.

- **The Independent Fluctuation Assumption (IFA).** This condition states that the two terms appearing in the exponential of Eqn. 122 are statistically independent:

$$\beta\Gamma_{\tilde{\mathbf{Q}}^2}^{IZ} \approx \frac{1}{N} \ln \left\langle e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \tilde{\mathbf{A}}_N \mathbf{T}]} \right\rangle_{\tilde{\mathbf{A}}} \left\langle e^{\frac{N}{2} \ln(\det(\tilde{\mathbf{A}}_M))} \right\rangle_{\tilde{\mathbf{A}}}. \quad (123)$$

- **The Exact Renormalization Group Condition (ERG).** This condition states that the determinant of the Student (and Teacher) Correlation matrix is unity, such that:

$$\det(\tilde{\mathbf{A}}) = 1 \quad \text{or} \quad \text{Tr}[\ln \tilde{\mathbf{A}}] = 0, \quad (124)$$

(and with  $\mathbf{A}$  additionally normalized to  $M$ , as explained in the Appendix, Section A.2.1) so that when we replace the measure over Student layer weight matrices  $d\mu(\mathbf{S})$  with a measure over all Student Correlation matrices  $d\mu(\mathbf{A})$ , *restricted to the ECS*, the second term in Eqn. 123 becomes unity,  $\langle \exp[\frac{N}{2} \text{Tr}[\ln[\det \mathbf{A}_M]]] \rangle_{\tilde{\mathbf{A}}} = 1$ , and vanishes in the final expression for  $\beta\Gamma_{\tilde{\mathbf{Q}}^2}^{IZ}$ .

At this point, the IFA is made purely for mathematical convenience, i.e., we have not demonstrated it empirically, but it is not implausible as a statistical modeling assumption. On the other hand, we can test the ERG condition empirically; this is a critical part of our SETOL approach.

Notably, when taking the large- $N$  approximation of  $\beta\Gamma_{\tilde{\mathbf{Q}}^2}^{IZ}$ , we effectively do this independently in two steps. First, we apply a Saddle Point Approximation (SPA) to the second term in Eqn. 123, leading to the ERG condition (see Appendix A.4). Most importantly, we can test the ERG condition empirically, and this is another critical part and justification of our SETOL approach. Second, when applying the result by Tanaka (Eqn. 75), we are applying an SPA to the result, but assuming we are restricted to the ECS.

**Empirical Tests of the ERG Condition and the ECS.** Since we require that the students resemble the fixed Teacher, a reasonable estimate for the average of the Student Correlation matrix  $\tilde{\mathbf{A}}$  (either  $\tilde{\mathbf{A}}_M$  or  $\tilde{\mathbf{A}}_N$ ) (in the ECS) is the point estimate provided by the actual (known) fixed Teacher correlation matrix  $\tilde{\mathbf{X}}$ ,

$$\left\langle \det \tilde{\mathbf{A}}_M \right\rangle_{\tilde{\mathbf{A}}} = \left\langle \det \tilde{\mathbf{A}}_N \right\rangle_{\tilde{\mathbf{A}}} \simeq \det \tilde{\mathbf{X}} = \prod_t \lambda_t = 1 \quad \forall \tilde{\lambda}_t \in \rho_{tail}^{emp}(\lambda), \quad (125)$$

for all eigenvalues  $\tilde{\lambda}_t$  in  $\rho_{tail}^{emp}(\lambda)$  the tail of the ESD of  $\tilde{\mathbf{X}}$ , i.e.,  $\tilde{\lambda}_t \geq \tilde{\lambda}_{min}$ . How should one choose  $\tilde{\lambda}_{min}$  in this expression? We already know that most NNs layers have Fat-Tailed ESDs, but if the

<sup>36</sup>Also, we could replace  $\mathbf{T} \rightarrow \tilde{\mathbf{T}}$ , but to simplify the notation, we do not do this.

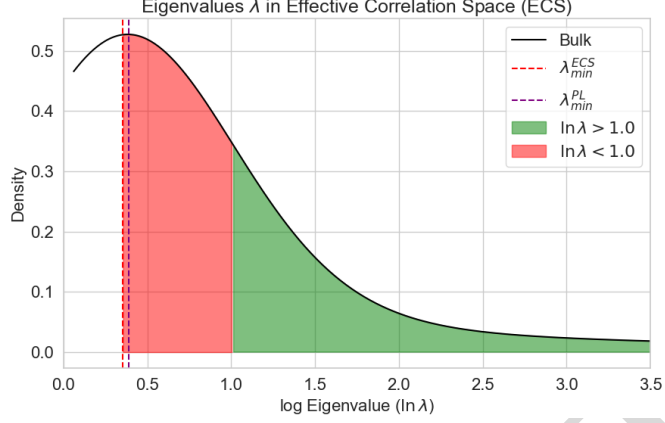


Figure 11: The image depicts a typical Empirical Spectral Density (ESD) of a layer correlation matrix  $\mathbf{X}$ , with **WeightWatcher** Power-Law (PL) exponent  $\alpha = 2.0$ . The green and red shaded regions depict eigenvalues  $\lambda$  in the Effective Correlation Space (ECS) of  $\tilde{\mathbf{X}}$ , defined by  $\lambda > \lambda_{min}^{ECS}$ . The x-axis displays the eigenvalues on the log scale,  $\ln \lambda$ . The vertical red line is at the start of the PL tail ( $\lambda_{min}^{PL}$ ). The purple, vertical line is at the start of the ECS tail ( $\lambda_{min}^{ECS}$ ). The green shaded region depicts those eigenvalues where  $\ln \lambda > 1.0$ , whereas the red shaded region depicts those eigenvalues where  $\ln \lambda < 1.0$ . The ECS is defined such that the Exact Renormalization Group (ERG) condition is best satisfied, i.e.  $\sum \ln \lambda = 0$  for  $\lambda \geq \lambda_{min}^{ECS}$ .

2091 Teacher ESD is simply *Random-Like* or even Bulk+Spikes, then the expected value  $\langle \det(\mathbf{A}_M) \rangle$   
 2092 itself of the determinant of a random full rank Student Correlation matrix  $\mathbf{A}_M$  might be well  
 2093 defined and easy to estimate, and we might not even need to define the lower rank ECS. Indeed,  
 2094 in these cases, the correlated eigencomponents, if they exist, may be buried in the bulk region of  
 2095 the ESD and not readily identifiable. Because  $\rho_{tail}^{emp}(\lambda)$  is Fat-Tailed and Power Law (PL), this  
 2096 poses some difficulty, we need to first define the Effective Correlation Space (ECS).

2097 Because the Teacher ESD is most likely MHT and PL, if we choose  $\tilde{\lambda}_{min} := \lambda_{min}^{ECS}$  too small,  
 2098 and the tail extends too far into the bulk region of the ESD, then for all practical purposes  
 2099  $\det(\tilde{\mathbf{X}}) \ll 1$ . On the other hand, if we choose  $\tilde{\lambda}_{min}$  too large, then we only capture very large  
 2100 eigenvalues, and for all practical purposes  $\det(\tilde{\mathbf{X}}) \gg 1$ . Therefore, if we set the scale of  $\tilde{\mathbf{X}}$   
 2101 appropriately, we can choose a  $\tilde{\lambda}_{min}$  such that  $\det(\tilde{\mathbf{X}}) = 1$ . In this case, by choosing  $\tilde{\lambda}_{min}$   
 2102 appropriately, we can estimate the expected value of  $\langle \det(\mathbf{A}_M) \rangle$  with an empirical point estimate  
 2103 over the Teacher Correlation matrix, which is unity.

$$|\det \tilde{\mathbf{X}}| \simeq 1; \quad \text{Tr}[\ln \tilde{\mathbf{X}}] = \ln |\det \tilde{\mathbf{X}}| \simeq 0. \quad (126)$$

2104 This expression can now be used in a practical calculation to define a low-rank subspace  
 2105 that both allows us to evaluate the HCIZ integral, and to identify, in principle, the generalizing  
 2106 components of the layer. We also refer to Eqn. 126 as the ERG condition, which is technically  
 2107 its empirical form. For example, Figure 5.2.4 depicts the eigenvalues in the ECS for a typical  
 2108 ESD with PL  $\alpha = 2.0$ . Notice that the start of the PL tail, ( $\lambda_{min}^{PL}$ ), is very close to the start of  
 2109 the ECS tail. ( $\tilde{\lambda}_{min}$ ), i.e.  $\Delta \lambda_{min} := \tilde{\lambda}_{min} - \lambda_{min}^{PL} \approx 0$ . Also, notice that while there are many large  
 2110 eigenvalues,  $\ln \lambda > 1.0$ , there are numerous small eigenvalues as well,  $\ln \lambda < 1.0$ , such that the  
 2111  $\sum \ln \lambda \approx 0$  for  $\lambda \geq \tilde{\lambda}_{min}$ . In other words, the red and green shaded areas have the same measure.  
 2112 Additional plots like Figure 5.2.4, generated with **WeightWatcher**, can be found in Section 6, in



Figure 21 as well as plots of  $\Delta\lambda_{min}$  vs. the WeightWatcher PL  $\alpha$  for several real-world examples, in Figures 22 and 23.

### 5.3 Evaluating the Layer Quality ( $\bar{Q}$ ) in the Large- $N$ Limit

To generate the Average Quality,  $\bar{Q}^2$ , we first take the Large- $\mathcal{N}$  limit of  $\beta\Gamma_{\bar{Q}^2}^{IZ}$  in  $N$ ,

$$\beta\Gamma_{\bar{Q}^2, N \gg 1}^{IZ} := \lim_{N \gg 1} \beta\Gamma_{\bar{Q}^2}^{IZ} = \lim_{N \gg 1} \frac{1}{N} \ln \langle \exp N\beta \text{Tr} \left[ \frac{1}{N} \mathbf{T}^\top \tilde{\mathbf{A}}_N \mathbf{T} \right] \rangle_{\tilde{\mathbf{A}}} \quad (127)$$

and then take the appropriate partial derivative, analogously to how we did for  $\bar{\mathcal{E}}_{gen}^{ST}$ ; see Section A.3 for more details. This gives (as in Eqn. 65)

$$\bar{Q}^2 := \frac{1}{\beta} \frac{\partial}{\partial n} \beta\Gamma_{\bar{Q}^2, N \gg 1}^{IZ} \underset{\text{high-}T}{\approx} \frac{1}{n} \frac{\partial}{\partial \beta} \beta\Gamma_{\bar{Q}^2, N \gg 1}^{IZ} \quad (128)$$

Notice that since we are at high-Temperature, it doesn't matter which partial derivative we take, and we expect both results to yield the same expression.

This HCIZ integral in Eqn. 127 can be evaluated (i.e in the Large- $\mathcal{N}$  limit in  $N$ ) using a result by Tanaka —provided the matrix  $\tilde{\mathbf{A}}_N$  is low rank, which holds when the ERG condition is satisfied. Thus, moving forward, we will assume an Effective Correlation Space (ECS) of rank  $\tilde{M}$ , where  $\tilde{\lambda}_{min}$  is the  $M^{th}$ -largest eigenvalue of  $\tilde{\mathbf{X}}$ , and defines the start of the ECS (and whatever branch-cut is necessary to integrate  $R(z)$ ).

Tanaka's result for the ECS can be expressed as:

$$\lim_{N \gg 1} \frac{1}{N} \ln \langle \exp (n\beta \text{Tr} [\mathbf{T}^\top \tilde{\mathbf{A}}_N \mathbf{T}]) \rangle_{\tilde{\mathbf{A}}} = n\beta \sum_{i=1}^{\tilde{M}} \mathcal{G}(\tilde{\lambda}_i), \quad (129)$$

where the sum now only includes the eigenvalues of  $\tilde{\mathbf{X}}$  (in the ECS),  $\beta = \frac{1}{T}$  is the Inverse Temperature,  $n$  is the size of the training dataset, and  $\tilde{\lambda}$  is an eigenvalue of  $\tilde{\mathbf{X}}$ , the Teacher Correlation matrix projected into the ECS space.  $\tilde{\mathbf{A}}_N$  is the  $N \times N$  form of the Student Correlation matrix, with  $N - M$  non-zero eigenvalues, and  $\mathbf{T}$  is the  $N \times M$  Teacher weight matrix (also effectively projected into the ECS, i.e.  $\mathbf{T} \rightarrow \tilde{\mathbf{T}}$  here).  $\mathcal{G}(\lambda_i)$  is the Norm Generating Function, defined below.<sup>37</sup> This gives

$$\beta\Gamma_{\bar{Q}^2, N \gg 1}^{IZ} = n\beta \sum_{i=1}^{\tilde{M}} \mathcal{G}(\tilde{\lambda}_i), \quad (130)$$

This gives a final expression for the Average Layer Quality (Squared)  $\bar{Q}^2$  as

$$\bar{Q}^2 = \sum_{i=1}^{\tilde{M}} \mathcal{G}(\tilde{\lambda}_i), \quad (131)$$

Note that  $\bar{Q}^2$  is independent of  $N$  and  $\beta$ , and, indeed, Eqn. 128 is an equality.

The average Quality (squared) can be expressed as a sum over Generating Functions  $\mathcal{G}(\lambda)$ , which depend only the statistical properties of the actual Teacher Correlation matrix  $\tilde{\mathbf{X}}$  (projected into the ECS). Each term in the sum,  $\mathcal{G}(\tilde{\lambda}_i)$ , takes the form

$$\mathcal{G}(\lambda) := \int_0^\lambda R_{\mathbf{A}}(z) dz \xrightarrow{\text{ECS}} \int_{\tilde{\lambda}_{min}}^\lambda R_{\tilde{\mathbf{A}}}(z) dz \quad (132)$$

<sup>37</sup>We use the notation  $\langle \dots \rangle_{\tilde{\mathbf{A}}}$  for expected value and placed  $\frac{1}{N}$  on the L.H.S. to help the reader compare this to the original expressions in [83, 84]. Also, in [83, 84],  $\beta = 1/2$ , but, in fact, if one inserts  $-\beta$  as an inverse temperature into the final expression, it simply factors out.

where  $R_{\tilde{\mathbf{A}}}(\tilde{\lambda})$  is the R-transform from RMT, and  $\tilde{\lambda}_{min}$  is the lower bound of the ECS spectrum. Importantly, the R-transform for a Heavy-Tailed ESD may have a branchcut at or near the start of the ECS (as explained in Section 5.4), so restricting the integrand to start at  $\tilde{\lambda}_{min}$  is critical.

Since we expect the best Student matrices to resemble the actual Teacher matrices, we expect the Student correlation matrix  $\tilde{\mathbf{A}}$  to have similar spectral properties to our actual empirical correlation matrices  $\tilde{\mathbf{X}}$ . That is, from the perspective of HTSR theory and the classification into 5+1 Phases of Training [25], we expect all the  $\tilde{\mathbf{A}}$  to be in the same phase as  $\tilde{\mathbf{X}}$  (and, in addition, to have the same PL exponent value). That is,

2146

2147 *We expect the R-transform of  $\tilde{\mathbf{A}}$  to have the same functional form as the R-transform of  $\tilde{\mathbf{X}}$ .*

2148

2149 If our (Teacher) NN weight matrix exhibits a HT PL, then the tail the ESD ( $\rho_{tail}(\lambda)$ ) of the Student and Teacher will both take the limiting form of a PL, with the same empirical variance  $\sigma^2$  and (critically) the same PL exponent  $\alpha$ :

$$\rho_{tail}[\tilde{\mathbf{A}}](\lambda) \sim \rho_{tail}[\tilde{\mathbf{X}}](\lambda) \sim \lambda^{-\alpha}. \quad (133)$$

2152

Up until this point, our derivation of  $\bar{Q}^2$  only depends on the ERG condition, irrespective of the exact functional form of  $R(z)$ , therefore the SETOL approach is tested by examining how well the ERG condition and the ECS holds for the layers in very well-performing models. We do this in Section 6.3.

2155

## 2156 5.4 Modeling the R-Transform

2157 To apply SETOL, the model must satisfy the ERG condition—which occurs during the case of Ideal Learning. For most cases of NN models, the ESD are HT; and in practice, one usually would select  $R(x)$  that reflects this. But to be more general, we formally extend the theory to allow the practitioners to both model the ESD as just a collection of discrete spikes, and to even correct for Correlation Traps and/or Very Heavy-Tailed (VHT) ESDs. Most importantly, we derive expressions for both the WeightWatcher Alpha and AlphaHat metrics, valid for the case Ideal Learning where  $\alpha = 2$ , and formally extended for other cases.

2164 The goal of this section is to obtain formal expressions for the Layer Quality,  $\bar{Q}$  which is given in terms of what we somewhat imprecisely refer to as a Norm Generating Function. In many cases, however, the resulting approximate expressions for  $\bar{Q}$  do take the form well-known norms, including the Frobenius norm, the Spectral norm, and the Shatten norm. The models for  $R(z)$  we use are presented in Table 8. The inal expression for the Layer Quality  $\bar{Q}$  extended *Semi-Empirically* to the non-ideal layers that can then be used to obtain the HTSR Alpha and AlphaHat metrics; these are given in Table 9.

### 2171 5.4.1 Elementary Random Matrix Theory

2172 We begin with some useful notions definitions from Random Matrix Theory. Using the ESD  $\rho(\lambda)$ , defined as

2173

$$\rho(\lambda) := \frac{1}{M} \sum_{i=1}^M \delta(\lambda - \lambda_i), \quad (134)$$

2174 we can express the *Greens Function* (or *Cauchy-Stieltjes* transform  $C(z)$ ) by<sup>38</sup>

$$G(z) = C(z) := \int d\lambda \frac{\rho(\lambda)}{z - \lambda}. \quad (135)$$

<sup>38</sup>Notice our naming and sign convention in Eqn. 135. We equate the Greens Function  $G(z)$  with the (positive) Cauchy-Stieltjes transform,  $G(z) = C(z)$ . Other works may use the opposite sign convention,  $G(z) = -C(z)$ .

From  $G(z)$ , we can recover the ESD,  $\rho(\lambda)$ , using the inversion relation

$$\rho(\lambda) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{\pi} \text{IM}(G(\lambda + i\epsilon)), \quad (136)$$

where IM is the imaginary part of  $G(z)$ , and where the  $\lim_{\epsilon \rightarrow 0^+}$  means to take the limit approaching from the upper half of the complex plane. The R-transform,  $R(z)$ , can be defined using the Blue function  $B(z)$

$$R(z) := B(z) - \frac{1}{z}, \quad (137)$$

where the Blue function  $B(z)$  [38] is the functional inverse of the Greens Function  $G(z)$ ,<sup>39</sup> satisfying

$$B[G(z)] = z. \quad (138)$$

By specifying the  $R(z)$  transform, we specify the complete ESD,  $\rho(\lambda)$ . Here, we are actually only interested in the tail of  $\rho(\lambda)$ . That is, we can given  $R(z) = R(z)_{tail} + R(z)_{bulk}$ , we only need  $R(z) \approx R(z)_{tail}$ .

Before moving forward, it is first necessary to demonstrate the R-transform  $R(z)$  exists for the power-law ESDs that arise in SETOL; this is shown in Appendix A.7. Specifically, it is shown that while the  $R(z)$  does not formally exist for a pure power-law (PL) tail with  $\alpha = 2$ , it does generally exist for *Truncated* power-law (TPL) tails, defined such that the domain is compact, i.e.,  $\lambda \in [\tilde{\lambda}_{min}, \tilde{\lambda}_{max}]$ .

#### 5.4.2 Known R-transforms and Analytic (Formal) Models

There are only a few known analytic results for the explicit R-transform  $R(z)$ . The ones we need are in Table 8. Below, we review some of them, explaining what ESD they correspond to, and what the resulting Norm Generating Function  $G(\lambda)$  would be if applied as a model  $R(x)$  here.

#### 5.4.3 Discrete Model: Bulk+Spikes, MHT, HT

Here, we consider modeling the tail ESD,  $\rho_{tail}(\lambda)$ , as a collection of discrete spikes  $\lambda_{spike}$ , where  $\lambda_{spike} \geq \tilde{\lambda}_{min}$ . This could be for modeling an ESD in the Bulk+Spikes (BS) HTSR Universality class, or it could be applied to an MHT or HT ESD as a discrete distribution with no inherent structure; its a modeling choice. Here, R-transform for the ECS is sum of Dirac delta functions. This lets us compute the Layer Quality  $\bar{Q}$  in closed form in terms of the Teacher weight matrix  $\mathbf{T} = \mathbf{W}$  as a Tail norm, the Frobenius norm of the tail eigenvectors.

Let the tail of the ESD have  $\tilde{M} = M^{tail}$  eigenvalues that define the ECS, i.e.,

$$\rho_{tail}(\lambda) = \sum_{i=1}^{\tilde{M}} \delta(\lambda - \tilde{\lambda}_i). \quad (139)$$

where the  $\tilde{\lambda}_i$  are normalized by  $\frac{1}{\tilde{M}}$ .

The Greens Function  $G(z)$  is then

$$G(z) = \int d\lambda \frac{\rho_{tail}(\lambda)}{z - \lambda} = \sum_{i=1}^{\tilde{M}} \int d\lambda \frac{\delta(\lambda - \tilde{\lambda}_i)}{z - \lambda} = \sum_{i=1}^{\tilde{M}} \frac{1}{z - \tilde{\lambda}_i}, \quad (140)$$

<sup>39</sup>The Blue function was first introduced by Zee [38] to model, among other things, spectral broadening in quantum systems. Briefly, given a deterministic Hamiltonian matrix  $\mathbf{H}_0$ , with eigenvalues  $\lambda_i^0$ , one can model the spectral broadening of  $\lambda_i^0$  by adding a random matrix  $\mathbf{H}_1$  to  $\mathbf{H}_0$ :  $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1$ . The resulting eigenvalues of  $\mathbf{H}$  now contain some level of randomness,  $\sigma$ , i.e.,  $\lambda = \lambda^0 + \sigma$ . To model the ESD of  $\mathbf{H}$ , one then specifies the R-transforms for  $\mathbf{H}_0$  and  $\mathbf{H}_1$ ; the full ESD of  $\mathbf{H}$  can then be reconstructed by adding the two R-transforms together  $R(z) = R_0(z) + R_1(z)$ . Zee notes that  $R(z)$  is the self-energy  $\Sigma(z)$  from quantum many body theory [38].

Model	HTSR Universality Class	$R(z)$
Discrete	Bulk+Spikes, MHT, HT	$\frac{1}{M} \sum_{i=1}^M \lambda_i$
Wishart Models		
Multiplicative-Wishart	HT/VHT	$\frac{\epsilon \phi z^2}{2 - \epsilon \phi^2 z^2}$
Inverse Marchenko-Pastur (IMP)	HT/VHT	$\frac{\kappa - \sqrt{\kappa(\kappa - 2z)}}{z}$
Lévy Wigner (LW)		
Free Cauchy (FC) ( $\alpha_l = 1$ )	HT $\alpha = 2$	$a + i\gamma$
General Lévy ( $\alpha_l \neq 1$ )	VHT $\alpha < 2$	$a + bz^{\alpha-2}$

Table 8: Known R-transforms for random matrix ensembles relevant to modeling heavy-tailed spectral densities (eigenvalues or singular values squared). The *Multiplicative-Wishart* model has two real, non-zero parameters,  $\epsilon$  and  $\phi$ ; for more details, see [111]. For the *Inverse Marchenko-Pastur*, as given by Bun [112],  $\kappa = \frac{1}{2}(Q - 1)$  where,  $q = \frac{1}{Q} = \frac{M}{N} \leq 1$ . The *Lévy-Wigner* (LW) model describes Wigner-like square random matrices (as opposed to Wishart-like or Correlation Matrices), where the elements are drawn from a Lévy-Stable distribution. The resulting LW ESD is Heavy-Tailed Power Law, and characterized by the Lévy exponent  $\alpha_l$ . The LW  $R(z)$  is parameterized by a (real) shift parameter  $a$ , a complex phase factor  $b$  (that depends on 3 real parameters  $\alpha_l, \beta$ , and  $\gamma$ ), and, of course,  $\alpha_l$ . The Free Cauchy (FC) model is a special case of the IW model, corresponding to the Lévy  $\alpha_l = 1$ , and the HTSR  $\alpha = 2$ . We will extend the LW models to the rectangular case for our modeling purposes here by making the association  $\alpha = \alpha_l + 1$  for  $\alpha \leq 2$ . (Also, we take the variance  $\sigma = 1$  for all models.) Generally speaking, the Lévy  $R(z)$  are more complicated; for more details, see [113, 114, 115].

2203 and the Blue function for each individual term  $i$  is  $\frac{1}{z - \tilde{\lambda}_i}$ , i.e.,  $B(z) = \tilde{\lambda}_i + \frac{1}{z}$ . Now, using the additive  
2204 property of the R-transform, we can express the total  $R(z)$  as the sum of the R-transforms for  
2205 the individual terms  $i$ , giving

$$R(z) = \sum_{i=1}^{\tilde{M}} \left( \left( \tilde{\lambda}_i + \frac{1}{z} \right) - \frac{1}{z} \right) = \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i. \quad (141)$$

2206 This gives the Norm Generating Function  $\mathcal{G}(\lambda)$  as

$$\begin{aligned} \mathcal{G}(\lambda) &= \int_{\tilde{\lambda}_{min}}^{\lambda} \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i d\lambda \\ &= \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i \int_{\tilde{\lambda}_{min}}^{\lambda} 1 d\lambda \\ &= \left( \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i \right) (\lambda - \tilde{\lambda}_{min}) \end{aligned} \quad (142)$$

2207 Seeing that  $\tilde{\lambda}_{min}$  is usually quite small, we make the approximation

$$\mathcal{G}(\lambda) \approx \left( \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i \right) (\lambda), \quad (143)$$

2208 which gives the Quality-Squared approximately as

$$\bar{Q}^2 = \sum_{i=1}^{\tilde{M}} \mathcal{G}(\tilde{\lambda}_i) \approx \left( \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i \right)^2. \quad (144)$$

2209 We now see that we can define  $\bar{Q} := \sqrt{\bar{Q}^2} = \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i$  is what we call a Tail Norm, the Frobenius  
2210 norm of the tail eigenvalues.

#### 2211 5.4.4 Free Cauchy Model ( $\alpha = 2$ )

2212 For the *Free Cauchy* (FC) model the R-transform is a constant

$$R(z)[\text{FC}] = a + i\gamma, \quad (145)$$

2213 where the shift parameter  $a > 0$  translates the FC spectrum (i.e. so it overlaps with the the Power  
2214 Law tail of the ESD), and the scale parameter  $\gamma > 0$  sets the tail width. We do not attempt to  
2215 fit  $a$  and  $\gamma$  to a real-world ESD here but rather simply use this model formally,

2216 Because  $R(z)$  is independent of  $z$ , the integral is straightforward:

$$\mathcal{G}(\lambda)[\text{FC}] = \int_{\tilde{\lambda}_{\min}}^{\lambda} R(z)[\text{FC}] dz = (a + i\gamma)(\lambda - \tilde{\lambda}_{\min}). \quad (146)$$

2217 As explained in Appendix A.6, when  $R(z)$  is complex, we keep the *Real* part  $\mathcal{G}(\tilde{\lambda}_i)$ , giving,

$$\Re[\mathcal{G}(\lambda)[\text{FC}]] = a(\lambda - \tilde{\lambda}_{\min}). \quad (147)$$

2218 To obtain a formal expression for **Alpha**, we make two approximations. First, we take the  
2219 lower cut-off to be near zero ( $\tilde{\lambda}_{\min} \approx 0$ ).

$$|\mathcal{G}(\lambda)[\text{FC}]|_{\tilde{\lambda}_{\min} \approx 0} \approx a\lambda \quad (148)$$

2220 Second, we assume the Layer Quality-Squared is dominated by the largest term in the sum:

$$\bar{Q}_{\text{FC}}^2 = \sum_{i=1}^{\tilde{M}} |\mathcal{G}(\lambda)[\text{FC}]|_{\tilde{\lambda}_{\min} \approx 0} = a \sum_i \tilde{\lambda}_i \approx a\lambda_{\max} \quad (149)$$

2221 For the Heavy-Tailed ESDs, we generally find that as  $\lambda_{\max}$  increases, the HTSR  $\alpha$  decreases.  
2222 Just for illustrative purposes, If we take  $\log_{10} \lambda_{\max} \sim \frac{1}{\alpha}$  (assuming  $\log_{10} \lambda_{\max} > 1$ ), and take the  
2223 square root of both sides, we obtain the desired result for the log Quality, namely, that it scales  
2224 inversely with  $\alpha$

$$\log_{10} \bar{Q}_{\text{FC}} \sim \frac{1}{\alpha} \quad (150)$$

2225 If we extend this formally beyond the Ideal case to  $\alpha \geq 2$ , we now can explain why the HTSR  $\alpha$   
2226 makes a good Layer Quality metric in deep networks, as smaller  $\alpha$  suggests higher quality layers  
2227 and therefore a higher overall model quality and/or accuracy.

#### 2228 5.4.5 Inverse Marchenko-Pastur Model of Ideal Learning

2229 For a more realistic model of a layer ESD, here, we consider the Inverse Marchenko-Pastur (IMP)  
2230 model [112]. The IMP model treats the ESD of  $\mathbf{X}^{-1}$  when the ESD of  $\mathbf{X}$  itself is MP. As a  
2231 parametric model, it can be quite effective at treating VHT and HT (or Fat-Tailed) ESDs,  $\alpha \leq 4$ ,  
2232 but works best when  $\alpha = 2.0$ . To do this, one simply considers  $\kappa$ , as an adjustable parameter

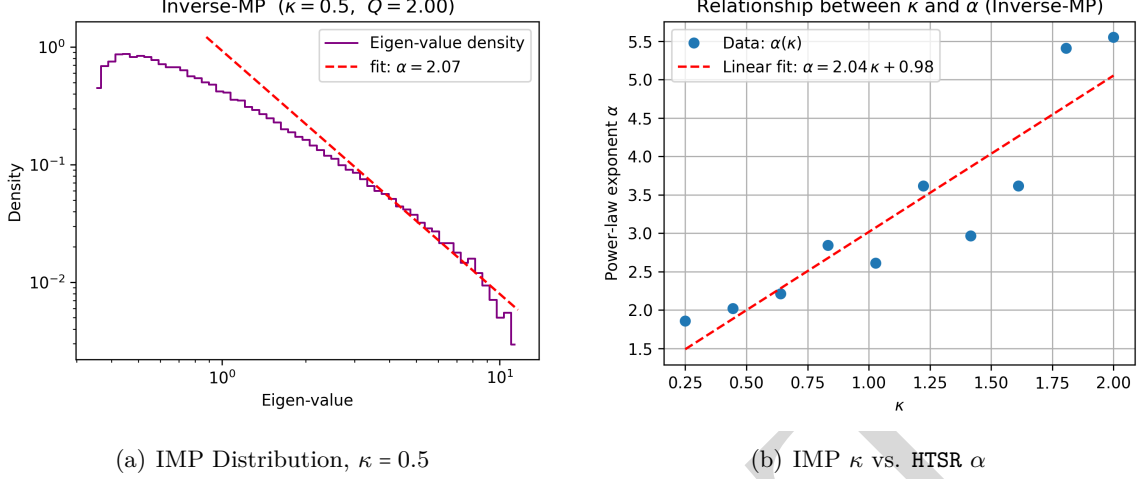


Figure 12: (12(a)) plots a typical Inverse Marchenko-Pastur (IMP) ESD  $\kappa = 0.5$ , along with Power Law (PL) fits, with PL exponent  $\alpha = 1.86$ . (12(b)) depicts the linear relationship between  $\kappa$  and  $\alpha$  for a few randomly generated examples.

which effectively captures the rank or soft-rank of an ECS-like space in these non-ideal layers. It is an excellent model for the ESD when  $\alpha = 2.0$  (and  $Q = 2$ ). Using this model, we can derive an expression for the HTSR AlphaHat Layer Quality metric,  $\hat{\alpha} := \alpha \log_{10} \lambda_{max}$  as a leading order term in the final expression for  $\log_{10} \bar{Q}^2$ .

In Figure 12, we generate a random IMP model ESD with  $\kappa = 0.5$ ,  $Q = 2.0$ , fit the ESD to a PL, and find  $\alpha = 1.08$ ; this is a reasonably accurate model of an PL ESD for  $\alpha \approx 2$ . For larger  $\kappa$ , the fits are not as good, but the model is still useful to suggest a heuristic model for the Layer Quality in terms of the HTSR  $\alpha$ . In Figure 12(b), we show that there is a simple relationship between  $\kappa$  and  $\alpha$ , which allows us to formally state  $\alpha = 2 \kappa$ .

Lets consider  $R(z)$  for the Inverse Marchenko-Pastur model, denoted  $R(z)[IMP]$ . To integrate this function, we require that it be analytic. At first glance, it may seem that that  $R(z)[IMP]$  is not analytic because it has a pole at  $z = 0$  and because the square-root term  $\sqrt{\kappa(\kappa - 2z)}$  creates branch cut at  $z = \kappa/2$  (and  $z = \infty$ ). Figure 13 presents this in two ways: Figure 13(a) shows the R-transform  $R(z)[IZ]$  for real  $z$ , highlighting its singular behavior and the location of the branch cut at  $z = \kappa/2$ ; and Figure 13(b) shows the corresponding branch cut in the ESD of the Inverse MP model (for  $\kappa = 0.5$ ). We select the branch cut starting at  $z = \kappa/2$  and ending at  $z = \infty$ , which allows us to at least formally defined the integral along the physically meaningful part of the ESD:

$$\mathcal{G}(\lambda)[IMP] := \int_{\tilde{\lambda}_{min}}^{\lambda} \Re[R(z)][IMP] dz, \quad (151)$$

noting that we expect  $\tilde{\lambda}_{min} \geq \kappa/2$  and we take the *Real* part of  $R(z)$ ,  $\Re[R(z)]$ .

It turns out, however, that due to the branch cut in  $R(z)[IMP]$ , the function  $\mathcal{G}(\lambda)[IMP]$  is not analytic in the domain we need. To correct for this, we will instead model the Layer Quality-Squared using the *Real Part*  $\Re[\mathcal{G}(\lambda)[IMP]]$ , which yields (See Appendix A.8):

$$G(\lambda)[IMP] = \int_{\tilde{\lambda}_{min}}^{\lambda} \frac{\kappa}{z} dz = \kappa [\ln z]_{\tilde{\lambda}_{min}}^{\lambda} = \kappa (\ln \lambda - \ln \tilde{\lambda}_{min}). \quad (152)$$

Notice this expression is very similar to the expression for the Free Cauchy model above (Eqn. 149),



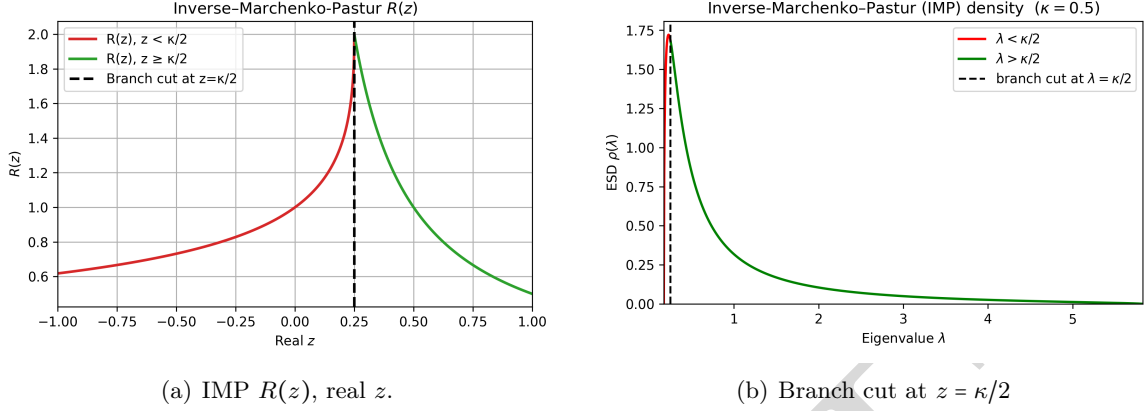


Figure 13: (a) The function  $R(z)$  of the Inverse Marchenko-Pastur (IMP) model, with a singularity at  $z = \kappa/2$ . (b) The branch cut in the Empirical Spectral Density (ESD) at  $\kappa = 0.5$ .

except now it is terms of the logarithm of  $\lambda$ , and rescaled by  $\kappa$ . By associating  $\alpha = 2\kappa$ , we recover the **AlphaHat** formular, albeit with a different normalization.

#### 5.4.6 The Multiplicative-Wishart (MW) model

The Multiplicative-Wishart (MW) model has two real, adjustable parameters  $\epsilon, \phi$ . It treats  $\mathbf{X}$  as resulting from a product of random matrices, and is good for modeling an ESD with a Very Heavy Tail (VHT). It has been used previously to model the heavy tail of the Hessian matrix in NNs [111]. This model would work better for fitting HT ESDs that decay slower than a PL or TPL. We note that unlike the IMP, the MW model does not have a branch cut at the ECS, but it does have 2 poles, complicating the integration of the R-transform. We will not consider this model further here and instead leave this for future work.

#### 5.4.7 Levy-Wigner Models and the AlphaHat Metric

Here, we consider General Levy-Wigner (LW) model.. We show how to obtain the **WeightWatcher AlphaHat** metric by modeling VHT ESDs with an approximation to a Levy distribution, suitable for cases where the HTSR  $\alpha \leq 2$ .

The **AlphaHat** metric has been developed to adjust for *Scale* anomalies that arise from issues like Correlation Traps, rank collapse, and overfitting, which can in many cases make **Alpha** smaller than expected, and even smaller than 2. We model these VHT ESDs *as if* they follow a Levy-Stable distribution, generated from a Levy-Wigner random matrix. The Levy-Wigner (LW) model treats  $\mathbf{X}$  as if it were a Wigner matrix (and not actually a rectnalgyle correlation matrix), s we must decide how to map the HTSR  $\alpha$  to the Lévy  $\alpha_l$ ; for this, we select  $\alpha_l = \alpha - 1$ . (See in Table 8.) The LW model is defined in terms of 3 parameters:  $a$  is a shift parameter, and  $b$  is a complex phase factor depending on 2 real factors,  $\beta$  and  $\gamma$ . Strictly the ESD for an LW model,  $\rho_{LW}(\lambda)$ , is defined by its characteristic function (i.e., the Fourier Transform of  $\rho_{LW}(\lambda)$ ), but when the ESD is VHT,  $\rho_{LW}(\lambda) \sim \lambda^{-\alpha_l-1}$ , and when  $\alpha_l \approx 1$ , the ESD resembles a PL HT ESD with the HTSR  $\alpha \approx 2$ .

Let us model the R-transform of our Very Heavy-Tailed (VHT) ESDs as

$$\begin{aligned} R(z)[\text{LW}] &= bz^{\alpha_l-1}, \alpha_l \in (0, 1) \\ &= bz^{\alpha-2}, \alpha \in (0, 2), \end{aligned} \tag{153}$$

where  $b$  is an unspecified constant (possibly negative and/or complex). This is not a particularly good model for VHT ESDs in practice; it is simply an approximate model, and we choose to obtain a formal expression.

Integrating  $R(z)[\text{LW}]$ , and (as above) taking the approximation  $\tilde{\lambda}_{\min} \approx 0$ , we obtain

$$\mathcal{G}(\lambda)[\text{LW}] \approx \frac{b}{\alpha-2} \lambda^{\alpha-2}. \quad (154)$$

For simplicity, if we now choose  $b = \alpha_l = \alpha - 2$ , then  $\bar{\mathcal{Q}}_{\text{LW}}^2$  takes the form of a Shatten Norm

$$\bar{\mathcal{Q}}_{\text{LW}}^2 = \frac{1}{M} \sum_i^{\tilde{M}} \lambda^{\alpha-1}. \quad (155)$$

Selecting the largest eigenvalue as the dominant term in the sum gives

$$\bar{\mathcal{Q}}_{\text{LW}}^2 \approx \lambda_{\max}^{\alpha-1}. \quad (156)$$

Taking the logarithm of  $\bar{\mathcal{Q}}_{\text{HT}}^2$ , we obtain

$$\log \bar{\mathcal{Q}}^2[\text{LW}] \approx (\alpha - 1) \log \lambda_{\max} \quad (157)$$

As with the Free Cauchy (FC), let us approximate  $\bar{\mathcal{Q}}^2$  by the largest term in the sum over  $\mathcal{G}(\tilde{\lambda}_i)$ , and then let  $\lambda = \lambda_{\max}$ , giving

$$\hat{\alpha} = \log_{10} \bar{\mathcal{Q}}_{\text{LW}}^2 \approx (\alpha - 1) \log \lambda_{\max}. \quad (158)$$

We present this as a formal example, noting that it is slightly different from the result for the IMP model. (See Table 9). We do not claim this is a valid empirical model, as we have not attempted to fit a real-world ESD to Levy-stable distribution. We leave this to a future study, noting however, there has been some work doing such fits [116].

Ideally, we would like to have a rigorous expression for  $R(z)$  not just in the case of Ideal Learning but also for the entire Fat-Tailed Universality class. This is nontrivial to obtain and we will attempt this in a future work. For now, we will take a different approach and evaluate  $R(z)$  explicitly using numerical techniques.

**Scaling insight.** For the VHT Universality class, we may expect  $\lambda_{\max}$  to be fairly large such that  $\lambda_{\max} > 1$  and therefore  $\log_{10} \lambda_{\max} > 0$ . This implies that  $\log_{10} \bar{\mathcal{Q}}^2$  decreases as  $\alpha$  (and thus  $\alpha_l$ ) decreases, even though  $\log_{10} \lambda_{\max}$  simultaneously *increases* in the VHT class. This opposing interplay explains why correlation traps produce small  $\alpha$  yet yield deceptively moderate quality scores.

**Historical remark.** An earlier study on AlphaHat, reported the opposite trend, with AlphaHat decreasing with increasing model quality. This is because we employed an un-normalized covariance, suggesting that  $\lambda_{\max} < 1$  and  $\log_{10} \lambda_{\max} < 0$  (although we have not rigorously checked this). The present  $M$  normalization clarifies that the VHT regime is meaningful *only* when  $\alpha < 2$ , indicating the layer and therefore the model is overfit (in some unspecified way).

#### 5.4.8 Summary of heuristic models.

Using the results for different R-transforms, we can construct several different, related heuristic models for the Layer Quality that resemble the very successful WeightWatcher HTSR Alpha and AlphaHat metrics. These heuristic models allow us extend the SETOL results for Ideal learning

Model	Tail Norm	WW Metric	$\log \mathcal{Q}$ (Log Quality)
Bulk+Spikes (BS)	Frobenius Norm	N/A	$\log \left( \sum_{i=1}^{\tilde{M}} \tilde{\lambda}_i \right)$
Free Cauchy (FC)	Spectral Norm	<b>Alpha</b> $\alpha$	$\log \lambda_{\max} \sim 1/\alpha$
Lévy Wigner (LW)	Shatten Norm	<b>AlphaHat</b> $\hat{\alpha}$	$(\alpha - 1) \log \lambda_{\max}$
Inverse Marchenko-Pastur (IMP)	ECS Boundary	<b>AlphaHat</b> $\hat{\alpha}$	$2\alpha[\log \lambda_{\max} - \log \lambda_{\min}]$

Table 9: Closed-form or leading-order expressions for the log Layer Quality  $\log \mathcal{Q}$  derived from the integrated  $R$ -transform for each core tail-model, simplified to show the relation to the **WeightWatcher** **Alpha** and **AlphaHat** metrics. For each model, we interpret the final result. Bulk+Space (BS): Sums the  $\tilde{\lambda}_i$  in the ECS, giving a Frobenius Tail norm. Free Cauchy (FC): Yields the Spectral Norm,  $\lambda_{\max}$ . Since this scales as  $1/\alpha$ , this explains the HTSR **Alpha** metric as it shows why smaller  $\alpha$  yields higher  $\mathcal{Q}$ . Lévy Wigner (LW): Yields a Shatten Norm, which can be approximated by **AlphaHat**,  $\hat{\alpha}$ . Being for the VHT Universality class, it implies that heavier tails ( $\alpha \in (1, 2)$ ) depress Layer Quality. Inverse Marchenko-Pastur (IMP): Also gives **AlphaHat**, and, importably, a branch cut that defines the ECS Boundary

(i.e.,  $\alpha = 2$ ) to a wider range of NN layers, covering the HTSR HT and VHT Universality classes and correspondingly, NN layers that are both underfit ( $\alpha > 2$ ) and overfit ( $\alpha < 2$ ).

Table 9 consolidates the derived expressions for the log Layer Quality,  $\log \mathcal{Q}$ , across multiple  $R$ -transform models, each capturing distinct heavy-tail characteristics of the ESD within the SETOL framework. The Discrete (Spikes) model yields a Frobenius-like tail norm by summing the effective eigenvalues in the ECS, directly tying quality to tail magnitude (cf. Eqn. 144). The Free Cauchy (FC) model links  $\log \mathcal{Q}$  inversely to the HTSR metric **Alpha**, demonstrating that smaller  $\alpha$  values enhance quality (cf. Eqn. 150). The Lévy-Wigner (LW) model connects  $\log \mathcal{Q}$  to **AlphaHat** through the term  $(\alpha - 1) \log \lambda_{\max}$ , revealing how very heavy tails depress layer quality (cf. Eqn. 158). The Inverse MP (IMP) model defines the ECS boundary via a branch cut at  $\kappa/2$  and approximates  $\log \mathcal{Q}$  as  $0.5 \log \lambda_{\max}$ , providing a robust metric for Ideal Learning scenarios. Each model thus offers a unique lens on layer quality, enabling direct mapping between theoretical  $R$ -transform assumptions and empirical **WeightWatcher** metrics.

**Practical Implications for Neural Network Analysis** These models empower researchers to tailor layer-quality assessments to specific HTSR universality classes, boosting the predictive power of **WeightWatcher** metrics like **Alpha** and **AlphaHat**. The Discrete model excels when the ESD exhibits clear eigenvalue spikes, delivering a sharp quality signal for Bulk+Spikes layers. The FC model supports Ideal Learning by linking quality directly to  $1/\alpha$ , which simplifies cross-layer comparisons. The LW model helps detect overfitting by adjusting for Correlation Traps via **AlphaHat** in very heavy-tailed regimes. Finally, the IMP model offers a parametric fit for both HT and VHT tails, with  $\kappa$  tuning alignment to real-world ESDs (cf. Figure 12). By integrating these models, practitioners can compute precise layer-quality metrics that optimize both performance and interpretability.

## 5.5 Computational Random Matrix Analysis

The R-transform is the generating function for the *Free Cumulants* of RMT. Formally—and if we assume a model without a branch-cut or troublesome poles—one can define  $R(z)$  as a series expansion in  $z$ ,

$$R(z) := \kappa_1 + \kappa_2 z + \kappa_3 z^2 + \dots \quad (159)$$

where the coefficients  $\kappa_k$  are the free cumulants, which can be expressed in terms of the matrix moments  $m_k$  [73], defined (here) as

$$m_k := \text{Tr}[\tilde{\mathbf{X}}^k] = \sum_{i=1}^{\tilde{M}} (\tilde{\lambda})^k \quad (160)$$

where  $\tilde{\lambda}_k$  is the  $k$ -th eigenvalue of the effective correlation matrix  $\tilde{\mathbf{X}}$ , which has been mean-centered and normalized by its standard deviation.

The free cumulants are defined recursively as

$$\kappa_k := m_k - \sum_{\text{partitions of } n \text{ blocks } B} \prod m_{|B|} \quad (161)$$

The first 5 *Cumulants* are, explicitly,

$$\begin{aligned} k_1 &= m_1 \\ k_2 &= m_2 - m_1^2 \\ k_3 &= m_3 - 3m_2m_1 + 2m_1^3 \\ k_4 &= m_4 - 4m_3m_1 - 2m_2^2 + 10m_2m_1^2 - 5m_1^4 \\ k_5 &= m_5 - 5m_4m_1 + 15m_3m_1^2 + 15m_2^2m_1 - 35m_2m_1^3 - 5m_3m_2 + 14m_1^5 \end{aligned} \quad (162)$$

Using these definitions, we can estimate the Layer Quality matrix  $\bar{\mathcal{Q}}^2$  for our experimental models (in Section 6 by computing  $\mathcal{G}(\lambda)$  for the effective correlation space (i.e., the tail of the layer ESD,) however it may be defined. That is, we use

$$\mathcal{G}(\lambda_i) = \kappa_1 \frac{\tilde{\lambda}}{\tilde{M}} + \frac{\kappa_2}{2} \left( \frac{\tilde{\lambda}}{\tilde{M}} \right)^2 + \dots \quad (163)$$

This is implemented in the `WeightWatcher` package. In Section 6.4, we examine some examples of this approach to computing Layer Qualities directly.

## 6 Empirical Studies

In this section, we present empirical results. Our goals are to justify key technical claims, including key assumptions underlying our SETOL approach, and to illustrate the behavior of SETOL with respect to various parameters and hyperparameters. Importantly, it is *not* our goal to demonstrate that layer PL exponent Alpha and AlphaHat perform well for diagnostics and predicting model quality for SOTA NN models, as that has been demonstrated previously [26, 24, 27].

Since the SETOL theory presented in Section 5 is (effectively) a single layer theory, in order to carefully test (as opposed to simply use) SETOL, we need to limit the degree of inter-layer interactions present in the model. To do so, we consider a three-layer Multi-Layer Perceptron (MLP3), trained on MNIST [117]. We refer to the hidden layers as “FC1 and “FC2. Their output sizes and parameter counts are shown in Table 10.

Layer	Units	Weight Parameters	% of total
FC1	300	$768 \times 300 = 230,700$	88.2%
FC2	100	$300 \times 100 = 30,000$	11.4%
out	10	$10 \times 100 = 1000$	0.38%

Table 10: Dimensions of each FC layer in the MLP3 model, along with weight matrix parameter count and fraction of the total.

The following are the main topics we consider.

**6.1 Model Quality: HTSR phenomenology.** The HTSR phenomenology provides a metric of model quality in the form of the PL exponent  $\alpha$ .<sup>40</sup> In particular, smaller values of  $\alpha$  (e.g., values of  $\alpha$  closer to 2 than 3 or 4) should correspond to better models, e.g., having smaller test errors; and a minimal error should be obtained when  $\alpha = 2$ . See Section 6.1.

**6.2 Effective Correlation Space.** The SETOL theory is based on the notion of an Effective Correlation Space, in which the learning and generalization occurs. This is the low-rank subspace  $\mathbf{W}^{ecs}$  of each layer  $\mathbf{W}$  that approximates the teacher  $\mathbf{T}$ . In particular, our measure of model quality should be restricted to  $\mathbf{W}^{ecs}$ . The Effective Correlation Space can be identified from the tail of the ESD,  $\rho_{tail}(\lambda)$ , and it can be chosen according to one of several related Model Selection Rules. See Section 6.2.

**6.3 Evaluating the ERG Condition.** In the HTSR phenomenology, when a model is very well-trained, the layer PL exponent  $\alpha \simeq 2$ . In the SETOL theory, when a model is very well-trained, the eigenvalues in the tail will satisfy the Empirical ERG Condition, given in Eqn. (126). In Section 6.3, we provide a detailed analysis of this effect.

**6.4 Computational Model Qualities.** In Section 6.4, we empirically compare the HTSR layer-quality exponent  $\alpha$  against the computational R-transform-derived metric  $\bar{Q}^2$  on fully trained MLP3 models. We show that for the FC1 layer,  $\bar{Q}^2$  closely tracks  $\alpha$  with small error bars and the expected batch-size trend, whereas for FC2,  $\bar{Q}^2$  exhibits much larger variability—demonstrating that  $\alpha$  provides a more stable and robust measure of layer quality.

**6.5 Correlation Traps.** Recall, from Section 3.3.1, that if a layer weight matrix  $\mathbf{W}$  has a Correlation Trap (and, in particular, those arising from SGD training with very large

<sup>40</sup>Prior work has shown that the AlphaHat metric ( $\hat{\alpha}$ ) accurately describes variations in model quality as a function of architecture changes [24]. Since we do not vary the depth of the model in our evaluations, the Alpha metric ( $\alpha$ ) is of interest in this setting.

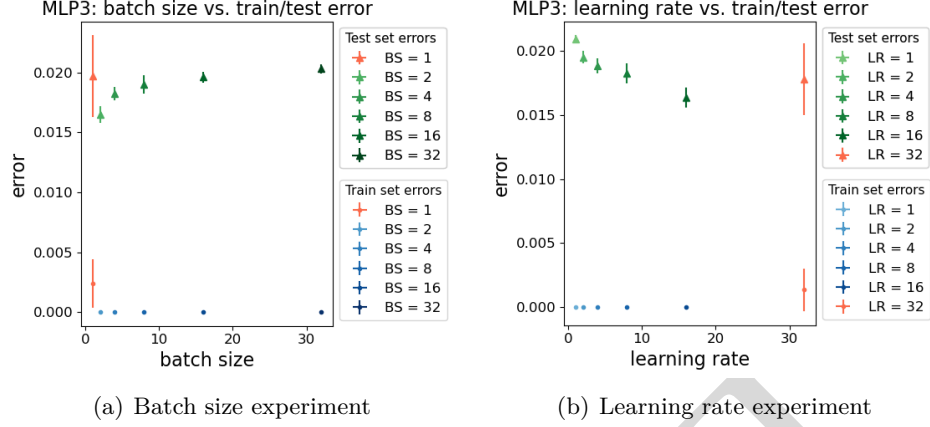


Figure 14: Train / test errors in the MLP3 model as a function of batch size, and learning rate. Observe the inverse relationship between batch size (a) and learning rate (b). As batch size decreases, test error generally decreases, until batch size reached  $bs = 1$ . Similarly, as learning rate increases, test error decreases until  $lr = 32\times$  the SGD default value of 0.01.

learning rates) then it is likely that the test (and train) accuracy will be degraded, and  $\alpha$  will drop below its optimal value. See Section 6.5 for an empirical demonstration of this.

**6.6 Overloading and Hysteresis Effects.** The experiments described so far validate that SETOL makes valid predictions in the  $\alpha \gtrsim 2$  range. Beyond that point, SETOL only predicts “atypicality, in the sense of spin glass theory [118]. See Section 6.6 for an examination of how the MLP3 behaves when it is pushed further out of that range of validity, e.g., by training only one layer, while keeping the others frozen. In particular, we compare results when a single layer is either over- vs under-parameterized.

We trained the MLP3 model independently, using both the Tensorflow 2.0 framework (using the Keras api, and on Google Colab) and pytorch, with the goal of consistent, reproducible results. Each setting of batch size, learning rate, and trainable layer was trained with 5 separate starting random seeds, and error bars shown in plots below represent one standard deviation taken over these 5 random seeds. Each training run used the same early stopping criteria on the train loss: training was halted when train loss did not decrease by more than  $\Delta E_{train} = 0.0001$ , over a period of 3 epochs. In doing so, each model was trained with a different number of epochs; and, at the end, the best weights were chosen for the model. See Appendix A.5 for more details on the MLP3 model and the training setup. We provide a Google Colab notebook with the exact details, allowing the reader to reproduce the results as desired.

The dominant generalizing components of  $\mathbf{W}$  reside in  $\mathbf{W}^{ecs}$  such that it captures the functional contribution of  $\mathbf{W}$  to the NN; and thus

## 6.1 HTSR Phenomenology: Predicting Model Quality via the Alpha metric

Here, we want to determine how the quality of our MLP3 model varies with the Alpha metric. From previous work [26, 24, 27], we expect that Alpha metrics for the FC1 and FC2 layers should be well-correlated with the test accuracy, while varying some suitable training knob, such as learning rate or batch size, that can modulate the test accuracy.<sup>41</sup>

<sup>41</sup>Since we do not change the depth of the model here, we expect the Alpha metric to follow the AlphaHat metric, also predicting the test accuracies [24].



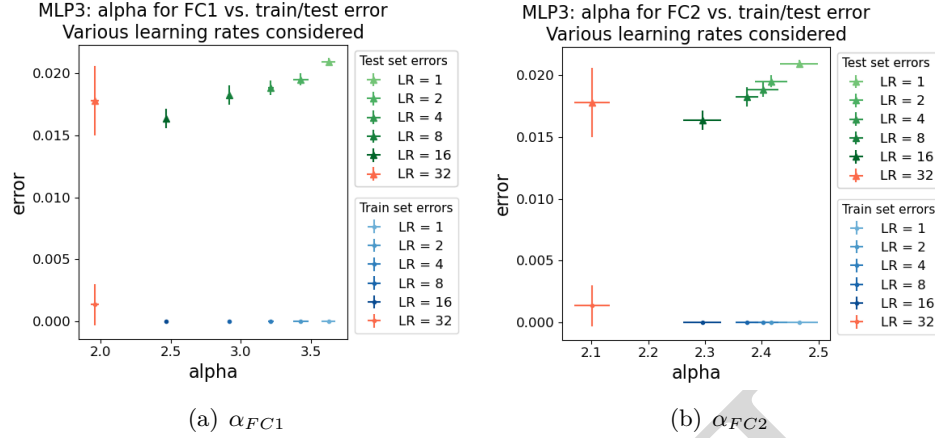


Figure 15: Train / test errors in the MLP3 model in the **Learning Rate** experiment as a function of  $\alpha_{FC1}$  (a) and  $\alpha_{FC2}$  (b). Observe the regular downward progression of  $\alpha$  and error as the learning rate increased in both (a) and (b). When learning rate was 32 $\times$ , (shown in red),  $\alpha_{FC1}$  fell below 2, coinciding with a drastic increase in both train and test error. The results here almost perfectly replicate those of the Batch Size experiment, shown in Figure 16. for Figure 16.

In doing this, the goal is not to achieve Thermodynamic equilibrium, but, instead, by using a common stopping rule, to simulate in more realistic situations where models may not have fully converged. This allows us to test the theory outside of its more limited apparent range of validity, thereby demonstrating the robustness of SETOL.

We vary the batch size from small to large, i.e.,  $bs \in [1, 2, 4, 8, 16, 32]$ , following the setup of previous work on the HTSR phenomenology [25]. We expect similar effects by varying the learning rate, as it is known that small batch sizes correspond directly to large learning rates [119, 120]. Thus, we conducted a second set of experiments where the learning rate was varied by a factor of  $[1\times, 2\times, 4\times, 8\times, 16\times, 32\times]$ , relative to the SGD default value of 0.01. Adjusting the learning rate or batch size allows us to systematically vary the layer PL exponent  $\alpha$  between roughly 2 and 4, i.e., within the range in which SETOL should make the most reliable predictions. As an added benefit, it also allows us to use the very small batch size of 1 to force the model into a state of over-regularization, which we also analyze below.

Consider Figure 14, which plots the final train and test accuracies as a function of the hyperparameter (batch size or learning rate) used during training for the MLP3 model. Figure 14(a) varies batch size, and Figure 14(b) varies learning rate. Recall that error bars represent one standard deviation taken over 5 independent starting random seeds. In Figure 14(a), we see that by decreasing the batch size ( $bs$ ), and holding other knobs constant, we can systematically improve the train and test accuracy, up to a point. In particular, for  $bs \geq 2$ , both the test and train accuracies increase with decreasing batch size, consistent with previous work [25]. Further decrease beyond  $bs = 2$  leads to *lower* model quality, i.e., larger error and larger error variability. In Figure 14, we see that increasing the learning rate ( $lr$ ) by a factor  $x$  has an exactly analogous effect as decreasing the batch size by  $1/x$ .<sup>42</sup>

The transition between  $lr = 16\times$  (or  $bs = 2$ ), which is locally optimal for the setting of other hyperparameters, and  $lr = 32\times$  normal (or  $bs = 1$ ), which is not, provides a demonstration of a distinct change in the behavior of Alpha, concordant with the sudden increase in the error and error variability. To explore this in the context of SETOL, consider Figure 15 and Figure 16, which

<sup>42</sup>One could, of course, mitigate this by fiddling with other knobs of the training process, but that is not our goal. Our goal here is not to use a toy model to demonstrate the properties and predictions of SETOL.

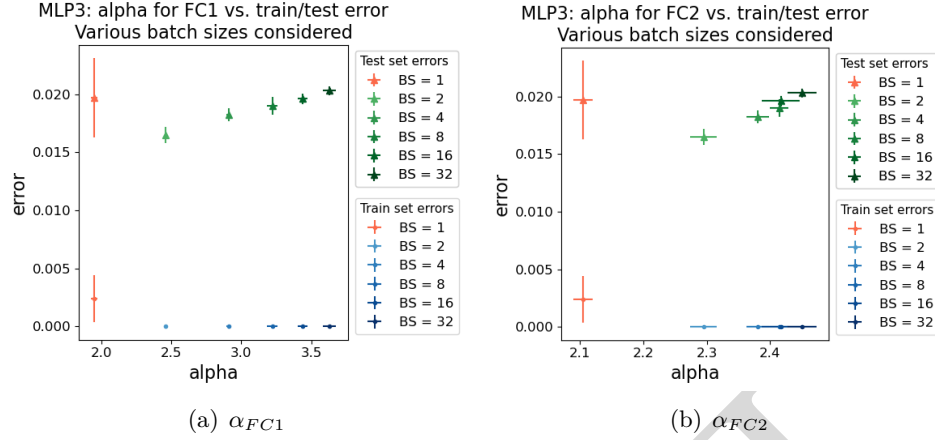


Figure 16: Train / test errors in the MLP3 model in the **Batch Size** experiment as a function of  $\alpha_{FC1}$  (a) and  $\alpha_{FC2}$  (b). Observe the regular downward progression of  $\alpha$  and error as the batch size decreased in both (a) and (b). When batch size was 1, (shown in red),  $\alpha_{FC1}$  fell below 2, coinciding with a drastic increase in both train and test error. The results here almost perfectly replicate those of the Learning Rate experiment, shown in Figure 15.

plot error as a function of **Alpha**, for different learning rates and batch sizes, respectively.

Figure 15 plots the **Alpha** metrics  $\alpha_{FC1}$  and  $\alpha_{FC2}$ , as learning rate is varied, demonstrating that both metrics are well-correlated with the test accuracies, for all learning rates less than  $16\times$  normal. In particular, as we drive **Alpha** in FC1 down to an Ideal value of  $\alpha \simeq 2$ , the test error decreases monotonically (Figure 15(a)). Beyond that point, further decrease of the batch size sees **Alpha** decrease below its Ideal value of 2 in the FC1 layer. This corresponds not only with *higher errors*, but also with *larger error bars*, on both train and test error. The dramatic increase in train error and train error variability is particularly telling, because it suggests that when  $\alpha_{FC1}$  passes below 2, the model enters into a “glassy state, and is unable to relax down to 0 train error.

In Figure 15(b), we consider **Alpha** for FC2, and we see that  $\alpha_{FC2}$  approaches 2, but does not reach it, even for  $lr = 32\times$ . This failure to achieve  $\alpha_{FC2} \approx 2$ , along with the much greater size of FC1, (See Table 10,) suggests that FC1 is the critical layer for the models performance. This also highlights some of the interplay between the layers, (which is not captured by a single layer theory) – as  $\alpha_{FC1}$  has narrow error bars throughout,  $\alpha_{FC2}$  shows much more variation by way of its wider error bars. Thus, while model accuracy kept improving as learning rate increased up to  $16\times$ , this was likely driven by a better  $\alpha_{FC1}$ , more than by  $\alpha_{FC2}$ .

In Figure 16, we consider batch size, and we see a near identical replication of these results, in terms of the relation of train error, test error and **Alpha** in the two layers. Consequently, the remainder of the experiments will focus on the learning rate experiment, as both produced substantially the same results.

## 6.2 Testing the Effective Correlation Space

Here, we will address the question:

How shall we *test the assumption* of the Effective Correlation Space?

Recall that the SETOL theory estimates model quality by evaluating the ST Generalization Error as an integral over the theoretical training data  $\xi$ . This integral assumes each layer weight matrix can be replaced with an effectively lower rank form, i.e.,  $\mathbf{W} \rightarrow \mathbf{W}^{ecs}$ , corresponding to the span

of the eigenvectors defined by the tail of the ESD,  $\rho_{tail}(\lambda)$ . In the HTSR phenomenology, the tail is defined by the fact that  $\rho_{tail}(\lambda)$  follows a PL distribution, above some minimal value  $\lambda_{min}$ . In our SETOL theory, the tail is defined by choosing the minimal value  $\lambda_{min}$  to satisfy the Empirical ERG condition. These methods of realizing  $\mathbf{W}^{ecs}$  are essentially *Model Selection Rules* (MSRs) for the Effective Correlation Space. Importantly, in neither approach is  $\lambda_{min}$  just some “rank parameter to be chosen by yet some other MSR on the basis of rank, or magnitude alone, (that, in particular, does not know about HTSR or SETOL, which consider the *shape* of the ESD).

Thus, to test the assumption of the Effective Correlation Space, we want to show that the models predictions are in fact controlled predominantly by the tail, where the specific choice of the rank parameter depends on HTSR or SETOL as we expect. We can emulate this theoretical construct and estimate (trends in the) test accuracies by evaluating the train and/or test accuracies of the trained MLP3 model – after replacing the MLP3 layer weight matrices  $\mathbf{W}_{FC1}$  and  $\mathbf{W}_{FC2}$  with a low-rank approximation consisting of *only* the tail:

$$\begin{aligned}\mathbf{W}_{FC1}^{ecs} &:= P_{tail} \mathbf{W}_{FC1} \\ \mathbf{W}_{FC2}^{ecs} &:= P_{tail} \mathbf{W}_{FC2},\end{aligned}$$

where  $P_{tail}$  is a projection operator selecting only the tail of the ESD with TruncatedSVD. (That is, we will use the low-rank TruncatedSVD approximation at the inference step, not at the training step, as is more common.) A Truncated model is one whose weight matrices  $\mathbf{W}_*$  have been replaced by truncated matrices  $\mathbf{W}_*^{ecs}$ . We denote the difference between the original models accuracy and the Truncated models train and test accuracy as  $\Delta E_{train}$  and  $\Delta E_{test}$ , respectively:

$$\begin{aligned}\Delta E_{train} &:= E_{train}(\mathcal{D}) - E_{train}^{ecs}(\mathcal{D}) \\ \Delta E_{test} &:= E_{test}(\mathcal{D}) - E_{test}^{ecs}(\mathcal{D}),\end{aligned}$$

where  $E_{train}^{ecs}$  denotes the error of the TruncatedSVD model on the training portion of the dataset  $\mathcal{D}$ , and  $E_{test}^{ecs}$  denotes corresponding test error for the TruncatedSVD model.

**The PowerLaw and ERG Model Selection Rules** If we use good MSRs, then we expect that  $\Delta E_{train} \rightarrow 0$  and  $\Delta E_{test} \rightarrow 0$  as the models approach Ideal Learning. We consider the following MSRs,<sup>43</sup> which are associated with the HTSR and SETOL approaches.

- The PowerLaw MSR: All eigenvalues lying in the tail of the ESD,  $\lambda_i \geq \lambda_{min}^{PL}$ , where  $\lambda_{min}^{PL}$  is the start of the PL tail, as determined by the WeightWatcher PL fit, which is based on [68].
- The ERG MSR: All eigenvalues lying in the tail of the ESD, such that they satisfy the ERG Condition, i.e.,  $\lambda_i \geq \lambda_{min}^{|detX|=1}$ , where  $\prod_{i:\lambda_i \geq \lambda_{min}^{|detX|=1}} \lambda_i \simeq 1$ .

### 6.2.1 Train and test errors by epochs

To see how the Effective Correlation Space forms, we plot how  $\Delta E_{train}$  and  $\Delta E_{test}$  evolve over training, for each of the various learning rates considered.<sup>44</sup>

We start with the effect of the PowerLaw MSR. See Figure 17, where we see that  $\Delta E_{train}$  and  $\Delta E_{test}$  generally trend downwards as they approach minimum train error. When the learning rate is larger, the models converge more quickly, and  $\Delta E_{train}$  and  $\Delta E_{test}$  also converge to lower

<sup>43</sup>We considered other MSRs that do not “know about HTSR or SETOL, but they (expectedly) perform in trivial or uninteresting ways for testing the assumption of the Effective Correlation Space. Thus, we are not introducing just some arbitrary low-rank approximation, as is common, but instead that the specific SETOL-based MSR matters.

<sup>44</sup>When batch size was varied, results did not significantly differ, and so they are omitted.

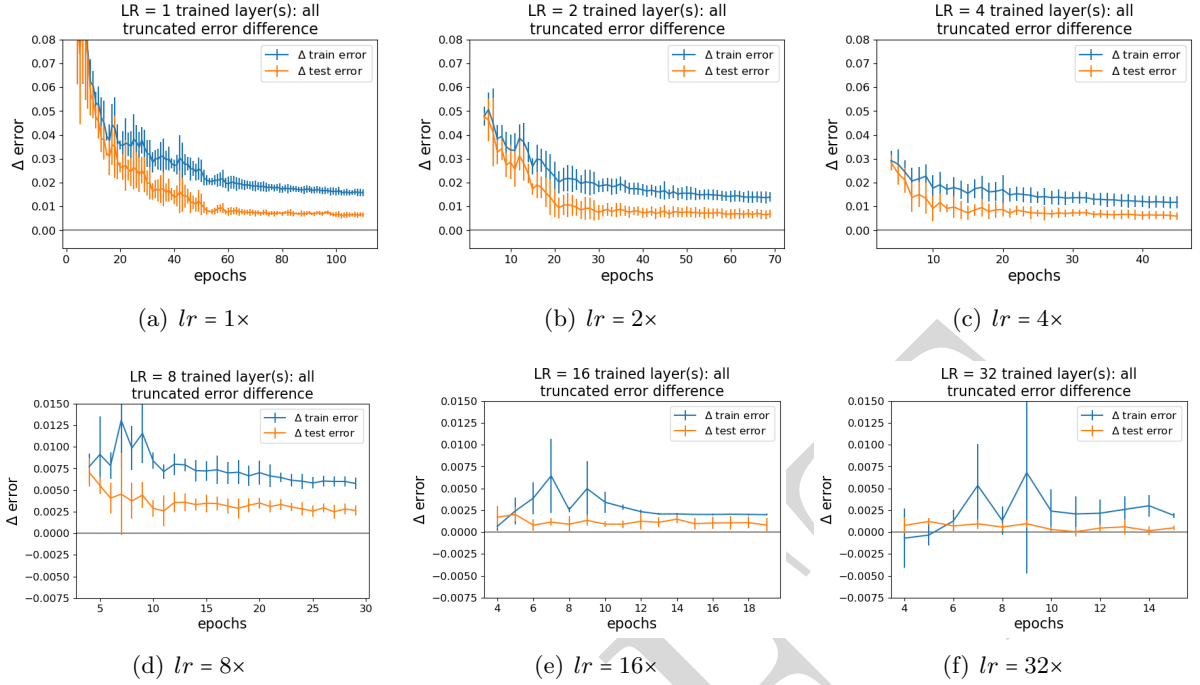


Figure 17:  $\Delta E_{train}$  (blue) and  $\Delta E_{test}$  (orange) for various learning rates, using the PowerLaw MSR. As learning rate increases we can see that  $\Delta E_{train}$  and  $\Delta E_{test}$  both tend towards lower asymptotic minima, which they reach after fewer epochs of training. We can also see that (after the first few epochs,)  $\Delta E_{train}$  (blue) is always higher than  $\Delta E_{test}$  (orange). Observe that in the bottom row (d–f) the yaxis is contracted to make the variation more visible. In (f) we can see that as learning rate surpasses its optimal setting, the gap between  $\Delta E_{train}$  and  $\Delta E_{test}$  begins to increase again, and has wider error bars, suggesting that the excessively large learning rate is disrupting the MLP3s ability to learn the Effective Correlation Space.

values. Recall from Figure 14(b) that  $lr = 16\times$  had the lowest test error. In Figure 17(e), we see that it also has the lowest  $\Delta E_{train}$  and  $\Delta E_{test}$ . A lower  $\Delta E_{train}$  or  $\Delta E_{test}$  means that more of the models correct predictions are due to the low rank tail, meaning that the tail generalizes better, and we see here that when the tail generalizes best, the model was the most accurate.

In each plot, we also see that the error bars are wide early on, before suddenly becoming much narrower. This transition is more visible in the larger learning rates shown in 17(d)–17(f), but can also be seen in 17(a)–17(c), albeit less clearly. Most interestingly of all, this transition is preceded by a brief period, sometimes a single epoch, in which the error bars are drastically wider, in a way that is reminiscent of a first-order phase transition. Again, this phenomenon can be seen most clearly in 17(d)–17(f).

We next consider the effect of the ERG MSR. See Figure 18, which also shows the development of  $\Delta E_{train}$  and  $\Delta E_{test}$  over epochs, where we see a very different pattern in the train error and test error. The difference in the train error is because, as the model is untrained in the early epochs, the ERG MSR *over*-estimates the tail by choosing a  $\lambda_{min}$  that is too small. Thus,  $\Delta E_{train}$  actually increases to its asymptotic value at the final epoch. In the earliest epochs, the truncated train error is even *less* than the full MLP3 models error, suggesting that signal is forming in the large eigenvalues in these early epochs, but is swamped by the randomness of the early initial weights, some of which is then removed by truncation. As epochs progress, this effect disappears. Here again we can see the “phase-transition-like behavior of the train error, as the error bars are

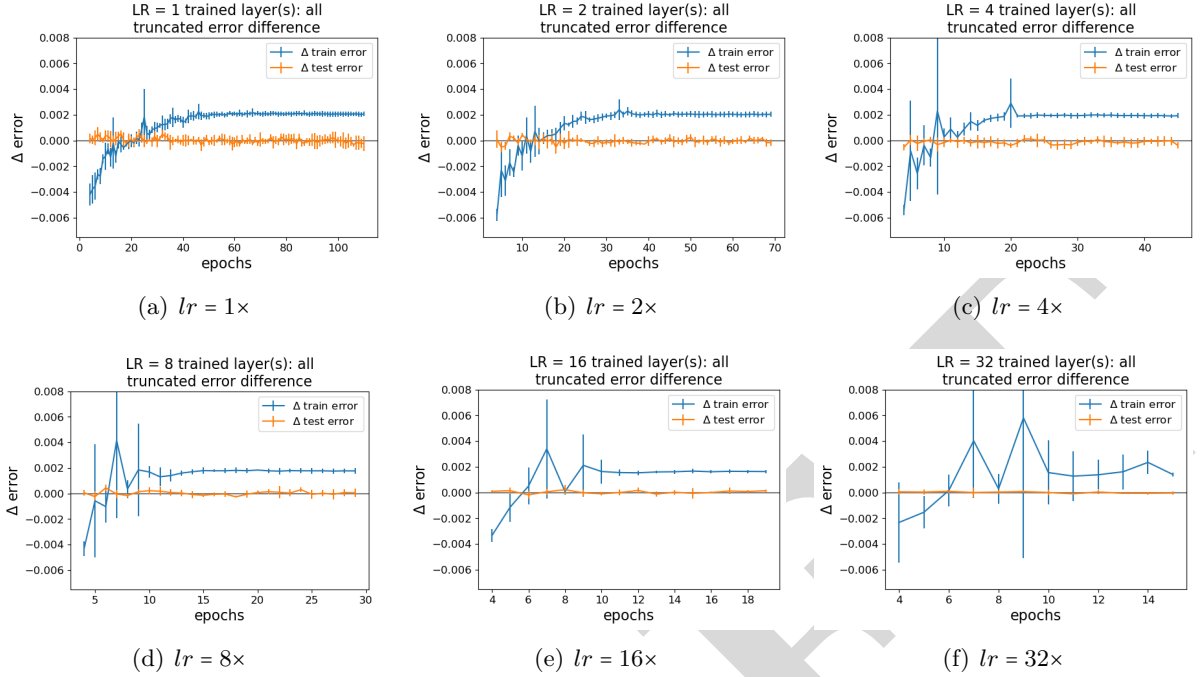


Figure 18:  $\Delta E_{train}$  (blue) and  $\Delta E_{test}$  (orange) for selected learning rates, using the ERG MSR. For all learning rates,  $\Delta E_{test}$  is centered on 0, meaning that the ERG Effective Correlation Space explains almost all variation in out-of-sample predictions, but it does *not* explain all of the training set predictions (blue). NOTE: The y axis is the same in all plots, and is much narrower than in Figure 17. In (a–e) we can see that  $\Delta E_{train}$  converges to approximately 0.002. Compare with Figure 17(e), which reaches a minimum of approximately 0.0025. As in Figure 17(f), the learning rate of 32 $\times$  normal disrupts the MLP3s ability to discover the ERG Effective Correlation Space.

wide early on, up to a transition having an abnormally large error bar, after which they stabilize.

Perhaps most interestingly of all, we see that under the ERG Model Selection Rule (MSR),  $\Delta E_{test}$  is flat *throughout training*, and for all learning rates. This implies that there is *no* point in training where the ERG tail generalizes badly. In other words, almost none of the out-of-sample variance falls outside of the Effective Correlation Space, as the ERG MSR over-estimates the Effective Correlation Space. It bears noticing that under the PowerLaw MSR, (Figure 17,) this is decidedly not the case, because the PowerLaw MSR *under*-estimates the Effective Correlation Space. As we will see in 6.3, as Alpha approaches 2, the gap between the two MSRs goes to 0.

There are two final points of comparison between Figures 17 and 18. First, although it appears in Figure 18 that  $\Delta E_{train}$  converges to a larger value than in Figure 17, this is because the scale of the y-axis is 10 $\times$  smaller. That is, the PowerLaw MSR is biased towards over-estimating  $\lambda_{min}$ , which means it over-truncates, producing a larger  $\Delta E_{train}$  or  $\Delta E_{test}$  than the ERG MSR, which is biased towards under-estimating  $\lambda_{min}$ . Second, in both Figure 17 and 18, we can see that  $\Delta E_{test}$  is consistently lower than  $\Delta E_{train}$ . Clearly, truncating has a larger effect on train predictions, meaning that no matter how long the model is trained, some of the train predictions are still derived from the bulk. The fact that they remain is evidence that the gradient does not degrade them, meaning that they were most likely contributing spuriously correct answers. Yet, the test predictions are far less affected, meaning that only the Effective Correlation Space contributes to the models ability to generalize.



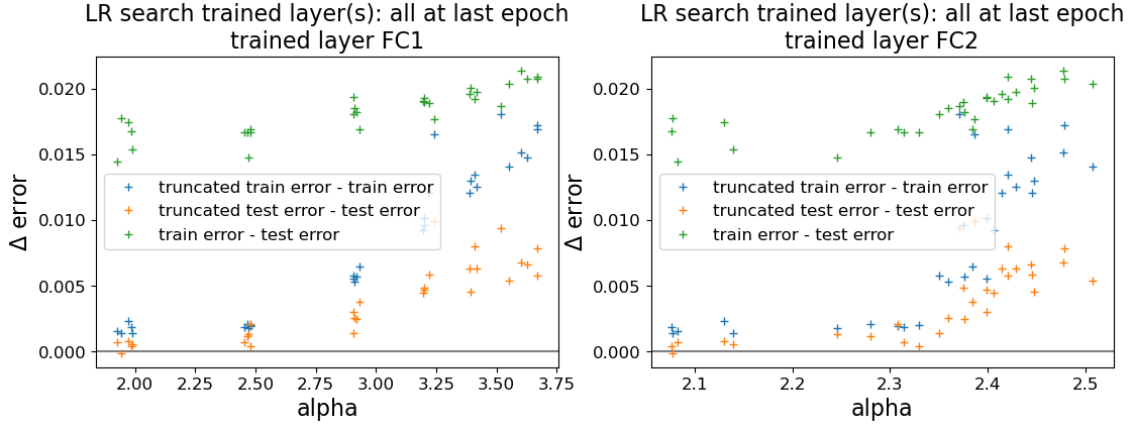


Figure 19: Train and test error gaps using the **PowerLaw** MSR, as a function of  $\alpha$  in the FC1 and FC2 layers of MLP3 models, at the *final epoch* of training. We can see that as  $\alpha$  decreases towards 2, (right to left),  $\Delta E_{train}$  and  $\Delta E_{test}$  generally decrease as well, meaning that the closer **Alpha** is to 2, the more the Effective Correlation Space explains the train and test predictions. The gap between un-truncated train and test error, (Eqn.84,) decreases as well until  $\alpha_{FC1} < 2$ .

## 6.2.2 Truncation and Generalization

Given that  $\Delta E_{test}$  is always lower than  $\Delta E_{train}$  for the **PowerLaw** MSR, and similarly for **ERG** after a certain point in training, it is clear that the Effective Correlation Space has something to do with generalization. However, this leaves open the question of what role precisely **Alpha** plays. In Figure 19, we plot  $\Delta E_{train}$  and  $\Delta E_{test}$  with the **PowerLaw** MSR as a function of **Alpha** (rather than epochs) for layers FC1 and FC2, as well as the Generalization Gap— that is,  $E_{test} - E_{train}$ . (Recall Eqn. 84.) Learning rate is not explicitly shown, but its effect can be seen in the clusters of points that each learning rate generates.

In both layers,  $\Delta E_{train}$  and  $\Delta E_{test}$  steadily decrease with  $\alpha_{FC1}$ , until it passes below 2, after which the relation deteriorates somewhat. This is especially prominent in FC2. Recall from Figure 15, Section 6.1, that when  $\alpha_{FC1}$  passed below 2, the train error and test error both increased and exhibited larger variability. From this we interpret **Alpha** as a measure of *regularization* (which is consistent with its introduction as a measure of implicit self-regularization [25]). Regularization has the effect of keeping train and test accuracy closer together, and generally, as **Alpha** in the dominant layer decreases towards 2 from above, the train-test error gap decreases.

## 6.3 Evaluating the ERG Condition

Having established that the PL tail of the ESD, defined by eigenvalues above  $\lambda_{min}^{PL}$ , is a major factor in determining model quality in the MLP3 model, we now examine how well the **ERG** Condition compares with it. In particular, we demonstrate that when the tail of a layer ESD is described well by the **HTSR** phenomenology, i.e., when it is well-fit by a PL with  $\rho(\lambda)_{tail} \sim \lambda^{-\alpha}$ , with PL exponent  $\alpha \simeq 2$ , then the eigenvalues in the tail defined by the PL fit, i.e.,  $\lambda \geq \lambda_{min}^{PL}$ , also satisfy the **ERG** Condition of Eqn. 126—a *key assumption of the SETOL theory*. This is a rather remarkable empirical result that couples **HTSR** and **SETOL**; it has its basis in our **SETOL** derivation; and it provides the basis for an inductive principle that is based on the product of eigenvalues rather than an eigenvalue gap.

We can denote the eigenvalue that best fits the **ERG** Condition as  $\lambda_{min}^{|detX|=1}$ . Then, to measure



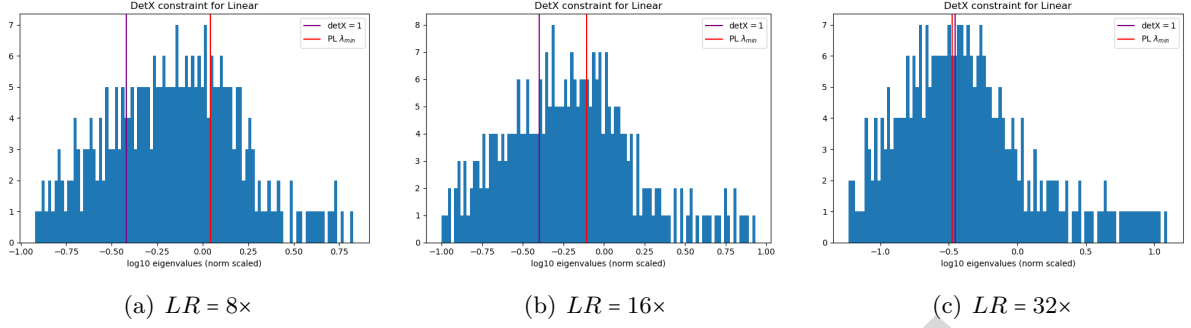


Figure 20: Log-Linear ESDs for three learning rates in the FC1 layer of MLP3. The red line shows  $\lambda_{min}^{PL}$ , and the purple line shows  $\lambda_{min}^{|detX|=1}$ . Observe that the purple line is to the left of the red line, but as the LR increases they move closer together. However, when LR is  $32\times$ , where both train and test accuracy suffered (c), the red line is to the left of the purple line. This is often a signature of an Over-Regularized layer, and indeed the FC1 layer in this model had  $\alpha < 2$ . (See Figure 15(a) in Section 6.1.)

how well this condition holds, we can compute

$$\Delta\lambda_{min} = \lambda_{min}^{PL} - \lambda_{min}^{|detX|=1}. \quad (164)$$

In Sections 6.3.1 and 6.3.2, we will see the trend that as  $\alpha$  approaches 2,  $\lambda_{min}^{PL}$  and  $\lambda_{min}^{|detX|=1}$  also approach one another, and hence  $\Delta\lambda_{min}$  goes to 0, from above, both for our toy MLP3 model as for SOTA models. In our MLP3 model, we will see that a crossing of the equality condition coincides with over-regularization and a degradation in model accuracy. In pre-trained ResNet[121], VGG[122] and ViT[123] models, we will also see, empirically, that in general  $\Delta\lambda_{min}$  remains positive, just as  $\alpha$  remains above 2.

### 6.3.1 The MLP3 model

Consider Figure 20, which shows  $\lambda_{min}^{PL}$  and  $\lambda_{min}^{|detX|=1}$  in the FC1 layer of three MLP3 models, each sharing a common starting random seed, that were trained with the largest learning rates. The  $\lambda_{min}^{PL}$  and  $\lambda_{min}^{|detX|=1}$  eigenvalues are marked by red and purple vertical lines, respectively; and thus  $\Delta\lambda_{min}$  is the distance between red and purple lines. As learning rate increases, the red and purple lines draw closer, and they are closest for  $lr = 32\times$  (Figure 20(c)). (Compare this with Figure 15, Section 6.1, which shows that this corresponds with an increase in test accuracy, up to  $lr = 16\times$ , but at  $lr = 32\times$  Alpha fell below 2 and accuracy suffered.) In Figure 20(a)-20(b), the purple line is left of the red line; but in Figure 20(c), the red and purple lines cross, such that  $\lambda_{min}^{PL} < \lambda_{min}^{|detX|=1}$ . This is analogous to the case where  $\alpha$  crosses below 2. This suggests that the absolute ERG is minimized when  $\alpha \simeq 2$ , which (remarkably) is exactly when the HTSR phenomenology predicts the layer is Ideal.

(Observe that Ideal does not necessarily mean optimal under a finite sized training set, but rather that the finite-sized system behaves the most similarly to its infinite limit.)

We can compare  $\alpha$  and  $\Delta\lambda_{min}$  more broadly by plotting  $\Delta\lambda_{min}$  directly as a function of  $\alpha$  in a single plot spanning all random seeds and learning rates or batch sizes. This is shown in Figure 21. Critical values of  $\alpha = 2$  and  $\Delta\lambda_{min} = 0$  are shown as vertical and horizontal red lines, respectively. Values for various learning rates are plotted for layer FC1 (Figure 21(a)) and FC2 (Figure 21(b)), as well as for various batch sizes in layer FC1 (Figure 21(c)) and FC2 (Figure 21(d)).

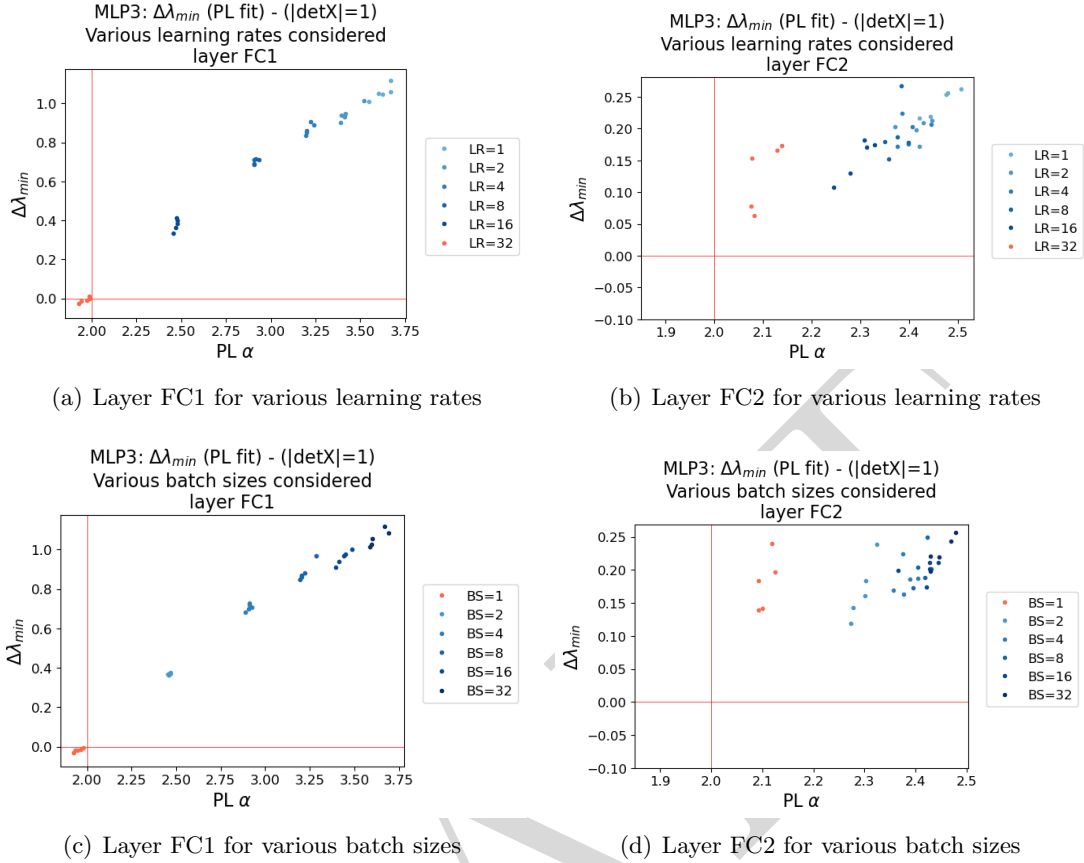


Figure 21: MLP3 Model: Comparison of the PL Alpha (x-axis), with the difference between  $\lambda_{min}^{PL}$  and  $\lambda_{min}^{|detX|=1}$  (y-axis). The thin red lines indicate critical values of  $\alpha = 2$  and  $\Delta\lambda_{min} = 0$ . As learning rate increases (a–b) or batch size decreases (c–d), we can see that in layer FC1, which dominates the model, (See Table 10,)  $\alpha$  goes to 2, and  $\Delta\lambda_{min}$  goes to 0. Observe that both critical values are crossed at the most extreme hyper-parameter selection, (red,) corresponding with over-training. Layer FC2 shows a weaker tendency towards the critical values (b, d), and is disrupted at the most extreme hyper-parameter values (red).

For layer FC1 (Figures 21(a) and 21(c)), in both cases we see near-linear march towards the critical tuple of  $(\alpha, \Delta\lambda_{min}) = (2, 0)$ . In addition, passing this critical value coincides with diminished train and test accuracy, (recall Figure 14), suggesting that just as  $\alpha = 2$  is a threshold of over-regularization,  $\lambda_{min}^{PL} < \lambda_{min}^{|detX|=1}$  may be as well. Since FC1 is the dominant layer, comprising roughly 8/9 of the weights of the model, (Table 10,) we expect FC1 to most closely match the performance of the model as a whole.

For layer FC2, which comprises roughly the other 1/9 of the models weights, there is a similar coevolution, but it is weaker. As learning rate or batch size exceeds their critical values, rather than going to  $(2, 0)$  as in FC1, we instead see that the relationship simply breaks down, with the gap growing larger even as  $\alpha$  decreases. Given that FC1 *has* passed the critical  $\alpha = 2$  threshold, we conjecture that the breakdown of the relationship between  $\alpha$  and  $\Delta\lambda_{min}$  is due to FC1 becoming atypical.

### 6.3.2 State-of-the-Art (SOTA) models

Here, we consider SOTA models, in particular VGG pre-trained models [122], the ResNet series [121], the ViT series [123], and the DenseNet series [124]. We show that as  $\alpha$  approaches 2, the Log-Trace Condition holds better and better, i.e.,  $\Delta\lambda_{min}$  approaches 0.

Figure 22 plots  $\alpha$  versus the difference  $\Delta\lambda_{min}$ , (Eqn. 164). Layer matrices from all models in each series are pooled to generate the plots.<sup>45</sup> Notice that in Figure 22(a) – 22(d),  $\Delta\lambda_{min}$  approaches zero as  $\alpha \rightarrow 2$  from above. Individual points may have a large  $\Delta\lambda_{min}$  for an  $\alpha$  near to 2, but the overall trend is apparent. The rapid decrease of  $\Delta\lambda_{min}$  as  $\alpha$  approaches 2 from above implies that the PL tail rapidly takes on a unit ERG (if it doesn’t already have it.)

As we saw in comparison of Figures 17 and 18, (Section 6.2.1,) the ERG tail is generally larger, and always has highly generalizing components. Thus, it is plausible that as layers reach the limit of the amount of information that can be encoded in them, i.e. as  $\alpha$  goes to 2, the PowerLaw tail expands to fill the ERG tail. This effect can be seen clearly in Figure 22 in the condensing of the “funnel shape.

Recall from Figure 21 that layer FC1 dominated the model, (Table 10,) producing a clear progression of  $\alpha$  and  $\Delta\lambda_{min}$  towards (2,0), as a function of learning rate or batch size, whereas FC2 showed a slightly less clear relationship. In larger models having dozens or hundreds of layers, we would not expect any one layer to dominate as thoroughly. Moreover, it is the architecture that varies between models in each series, not (necessarily) the hyperparameters, meaning that there would not be a straight line, as in Figures 21(a) and 21(c). However, with all of the layers contributing to varying degrees, we nevertheless see a clear trend in all plots of Figure 22. These results show how the single-layer SETOL theory extends from the MLP3 model, which is dominated by a single layer, to larger models where many layers interact in complex ways, but still reflect the same overall trend.

The overall pattern of relationship between  $\Delta\lambda_{min}$  and  $\alpha$  can also be seen in Figure 23, which shows plots for Large Language Models (LLMs) of the Falcon [125] and LLAMA [126] model families, for different numbers of parameters. Observe that each subfigure 23(a)–23(d) shows a single model, rather than a collection of models in a family, as in Figure 22. The y-axis is the same between models in the same family. As in Figure 22, there is a general outline of a “funnel shape pointing towards the critical point (2,0), with the exception that it is only reached in the case of LLAMA-65b, (Figure 23(d)). This suggests that these LLMs are larger than they necessarily need to be, consistent with prior work [80], but also that they are well guarded against Over-Regularized layers beyond the critical point ( $\alpha = 2$  and  $\Delta\lambda_{min} = 0$ ).

## 6.4 Layer Qualities with Computational R-transforms

In this Section, we look at how the HTSR layer quality HT PL metric  $\alpha$  compares to computing the Layer Quality-Squared  $\bar{Q}^2$  using the Computational R-transform method proposed in Section 5.5 for fully trained MLP3 model(s). Figure 24 presents results for FC1 and FC2 layers, comparing both the batch size and the mean  $\alpha$  metric to the mean  $\bar{Q}^2$ , and the results are quite different.

For FC1, as shown in Figure 24(a), the quality metric  $\bar{Q}^2$  increases as the batch size decreases, following the expected trend. Notably, for batch size = 1, the quality metric exceeds 100%, which suggests that the layer may be overfit in this scenario, which is similar to results obtained earlier. Furthermore, in Figure 24(b), the quality metric  $\bar{Q}^2$  shows a strong correlation with the  $\alpha$  metric,

<sup>45</sup>For convolutional layers, the WeightWatcher tool first computes eigenvalues for all channels-to-channels linear operators separately, and then pools them in order to compute  $\alpha$ ,  $\lambda_{min}^{PL}$  and  $\lambda_{min}^{detX=1}$ . For instance, in a  $64 \times 64 \times 3 \times 3$  weight tensor, there would be 9 separate linear operators of  $64 \times 64$ , giving 576 eigenvalues, which would then be pooled to compute  $\alpha$ ,  $\lambda_{min}^{PL}$  and  $\lambda_{min}^{detX=1}$ .

consistent with the theoretical predictions of the HTSR framework. Earlier results suggest that the FC1 layer captures most of the correlation in the data, so it is interesting that this layer also has much smaller error bars, indicating more consistent quality across different batch sizes.

In contrast, for FC2, while the general trends are similar (as shown in Figures 24(c) and 24(d)), the error bars on the quality metric  $\bar{Q}^2$  are much larger. This indicates significantly higher variability in computational quality compared to FC1. The large error bars for FC2 suggest that, while the  $\bar{Q}^2$  metric is theoretically grounded, it is less effective than the existing HTSR layer quality metric  $\alpha$ , which exhibits greater stability and reliability in capturing layer behavior. These differences highlight the distinct computational characteristics of the two layers, with FC1 demonstrating more predictable trends that align closely with theoretical expectations.

## 6.5 Inducing a Correlation Trap

Previous work on the HTSR phenomenology [26, 24] has shown that one can look for quantitative deviations from the necessary pre-conditions of traditional RMT (particularly that the weights are 0-mean and finite variance) to detect when a model layer suffers from some other anomaly in the elements, which we call a “Correlation Trap” (see Section 3.3.1 and [26, 24]). A Correlation Trap may cause, or be caused by, the over-regularization leading Alpha to fall below 2, (see Section 3.3.2). Here, we explore this in greater detail, in light of our SETOL.

Lets look at the ESDs of the FC1 layer of the MLP3 model, for learning rates  $lr = 16\times$  and  $lr = 32\times$  normal. We will be interested in the general shape of the ESD of  $\frac{1}{N}\mathbf{W}^T\mathbf{W}$ . For the purposes of detecting a Correlation Trap, we will randomize  $\mathbf{W}^T\mathbf{W}$  element-wise, and then observe its largest eigenvalue  $\lambda_{rand}^{max}$ .

Figure 25 shows the ESDs of the original matrix (green) and the element-wise randomized  $\text{rand}(\frac{1}{N}\mathbf{W}^T\mathbf{W})$  (red). Observe in particular  $\lambda_{rand}^{max}$  for each learning rate factor. For  $lr = 16\times$ , Figure 25(a) shows that the ESD of  $\frac{1}{N}\mathbf{W}^T\mathbf{W}$  is HT, whereas the ESD of the randomized matrix is essentially a distorted semi-circle—as expected from the well-known MP result; and that  $\lambda_{rand}^{max}$  lies at the edge of the random MP Bulk ESD. (A similar result is seen for smaller learning rates.) In contrast, for  $lr = 32\times$ , Figure 25(b) shows that while the original ESD is again HT, the ESD of the randomized has one large element,  $\lambda_{rand}^{max}$ , that pulls out from the MP bulk. This is the signature of a Correlation Trap; and it co-occurs with the exact learning rate setting that degraded the train and test accuracies, pushing Alpha below its optimal value of  $\alpha \simeq 2$ . When this happens, both the estimation of Alpha and the formation of a PL tail are potentially disrupted.

Correlation Traps have been observed previously [26, 24], using the HTSR phenomenology. However, SETOL provides an explanation for why this would be expected to occur — non-standard element-wise distributions will tend to interfere with the properties of the spectrum which SETOL analyzes. Our derivation in Section 6 suggests that in order to apply the SETOL effectively one must avoid (or remove) such traps. This too has been observed previously [26, 24].

## 6.6 Overloading and the Hysteresis Effect

Obtaining a value of  $\alpha$  outside the  $\alpha \gtrsim 2$  range is indicative of “overloading [8] that layer. This can be accomplished, e.g., by training only one layer in the MLP3 model. As the two layers have very different sizes, we see markedly different behaviors, that are nevertheless consistent with theory. In particular, this lets us test the theory in both the *Strongly Over-Parameterized Regime* ( $n \gg N \times M$ ) and the *Under-Parameterized Regime* ( $n \ll N \times M$ )

The SETOL theory is based on the idea that NNs undergoing training behave like Statistical Mechanic systems relaxing to an equilibrium. So far, we have tested the theory under conditions that are approaching Ideal. However, for the theory to be useful in practice, we must also

examine how it performs in non-Ideal situations. Of particular interest, we would like to examine the theory under conditions where the training dynamics slows down, i.e., when it is in a “glassy” or meta-stable state. One way we can do this is to train only one layer, and freeze the rest. Doing so overloads the single trainable weight matrix, as a function of the ratio of examples to trainable parameters [8, 6, 93], and we expect this to cause  $\alpha_{FC1}$  or  $\alpha_{FC2}$  to drop well below 2. As in 6.2, we will be examining this effect over the entire course of training.

### 6.6.1 Baseline: Loading onto both FC1 and FC2

To start, Figure 26 shows  $\alpha_{FC1}$  and  $\alpha_{FC2}$ , binned in units of 0.05, versus train and test error over all epochs of training<sup>46</sup> for each of the different learning rates considered. (Cf. Figures 15 and 16, Section 6.2, which show only the final epoch.) Binning was done so as to facilitate averaging over the 5 starting random seeds; linear fits are shown separately for each learning rate; and error bars represent one standard deviation within each bin. The critical value of  $\alpha = 2$  is shown as a vertical red line in all plots. For each learning rate, train error and  $\alpha$  decrease together during training, which can be seen for both  $\alpha_{FC1}$  (a) and  $\alpha_{FC2}$  (c), reading each line from the top right to bottom left. Test errors, (b, d) show a similar trend, but with wider error bars. Observe that the range of the y-axis is narrower for test error to make detail more visible.

We see in Figure 26 (a,b) that the  $32\times$  learning rate causes  $\alpha_{FC1}$  to decrease faster than any other, putting it on course to fall below 2 before train error reaches  $\simeq 0$ . (See Figure 14, at the beginning of this Section.) We also see that the slower learning rates cause train error to reach  $\simeq 0$  well before  $\alpha_{FC1}$  can reach 2, and explains as to why their test error was higher.

### 6.6.2 Overloading FC1: Strongly Over-Parameterized Regime ( $n \gg N \times M$ )

In contrast, when only FC1 is trained, Figure 27 shows that, as expected,  $\alpha_{FC1}$  decreases well below 2. Training error (a) generally trends downward as  $\alpha_{FC1}$  decreases, but no matter the learning rate, the relation is the same, or nearly so, because only one layer is being trained. Consequently, all learning rates were pooled to produce one linear fit for enhanced visibility.

In Figure 27 we can see demonstration of a crucial claim of SETOL theory: that for  $\alpha_{FC1} > 2$ , (vertical red line,) the test error declines linearly; (b) shows that test error is almost perfectly linear with decline in  $\alpha_{FC1}$ . However, when  $\alpha_{FC1} < 2$ , the curve bends upward. Furthermore, the precision with which the trajectory changes as  $\alpha_{FC1}$  passes the threshold provides ample validation that the estimator of [68] is indeed accurate. We observe that test error may continue to decrease after  $\alpha_{FC1} < 2$ , however the rate of decrease is significantly less. We can also see that in some sense, the model is “doomed” to always have train error reach  $\simeq 0$  when  $\alpha_{FC1} \simeq 1.7$ , i.e., after  $\alpha = 2$ , because of the number of trainable parameters, and perhaps because of the lack of a modulating influence of FC2 seen in Figure 26.

### 6.6.3 Overloading FC2: Under-Parameterized Regime ( $n \ll N \times M$ )

The MNIST dataset has 60,000 training examples, which means that an FC1-only model is over-parameterized, but FC2 is substantially *under*-parameterized [127]. (Table 10) This drastically changes the meaning of an experiment where only FC2 is trained. Figure 26 (Section 6.6.1) shows  $\alpha_{FC2}$  vs. train error (c) and test error (d) when *all* layers are trained. There we see a different relationship between  $\alpha_{FC2}$  and train and test error for each learning rate. None of the training runs reached an  $\alpha_{FC2}$  of 2, as the load was split between both layers FC1 and FC2.

<sup>46</sup>Excluding the first four epochs when the matrix is still essentially random.

Figure 28, however, shows a starkly different relationship. When only FC2 is trained, each random seed produces a different trajectory, meaning that they cannot be interpretably plotted as a single curve, even with error bars. Train (a, c) and test (b, d) error rates are shown as a function of  $\alpha_{FC2}$  for the two highest learning rate factors,  $16\times$  (a, b) and  $32\times$  (c, d). Lower learning rate factors, (not shown,) showed the same trend, except that they did not progress as far as those shown in Figure 28.

First we see, for all seeds,  $\alpha_{FC2}$  decreases all the way down to 1.5, after which it begins to rebound to the right. As it does, train error continues to decrease. We can also see that test error continues to decrease as well, down to its minimum value of slightly more than 0.03, as  $\alpha_{FC2}$  continues to increase for a short time. However, at the exact point where test error reaches a minimum, the PL tail itself begins to fracture, leading to different estimates of  $\alpha_{FC2}$  for each seed. As each of the five starting random seeds are shown separately, we can see that each of them terminates at a different point, some of which are closer to 2 than others.

Such a reversion to a more typical value of  $\alpha_{FC2}$ , prior to the fracturing of the PL tail, is reminiscent of a spin glass system relaxing towards its minimum energy configuration, in a way that retains some memory of the path taken on the way to its current state. We conjecture that if the model were trained for sufficiently many epochs, (perhaps many thousands,) then the tail would re-form, and  $\alpha_{FC2}$  would reform, and revert all the way back to its stable value of 2.



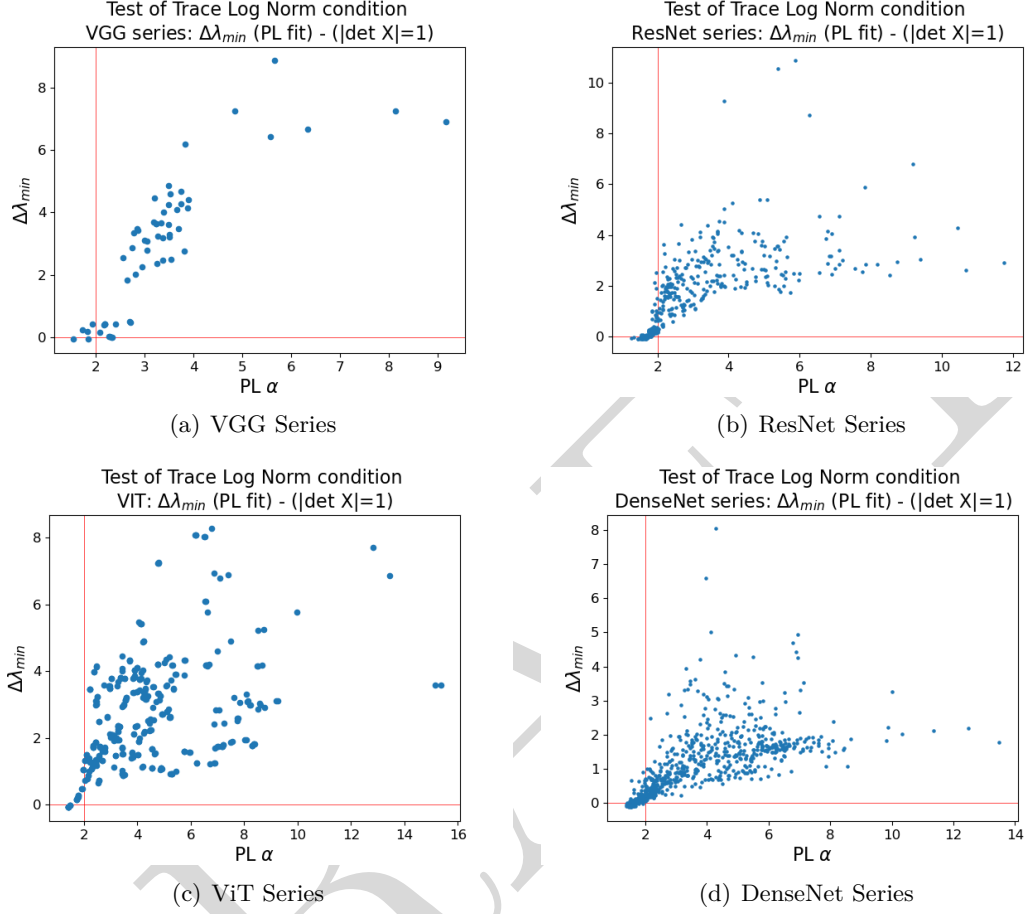


Figure 22: Difference between the two  $\lambda_{min}$  estimates,  $\Delta\lambda_{min}$ , (Eqn. 164), as a function of  $\alpha$ , for linear and convolutional layers in series of VGG [122], ResNet [121], ViT models [123] and DenseNet models [124]. Layer matrices for all models in the series were pooled to create each plot. In (a), (VGG,) we see three clusters of points – those with  $\Delta\lambda_{min}$  close to 0 and  $\alpha$  close to 2, those with  $\Delta\lambda_{min}$  above 2 and  $\alpha > 2.5$ , and those with  $\Delta\lambda_{min}$  above 6 and  $\alpha > 3.5$ . In (b), (ResNet,) we see that in general, as  $\alpha$  shrinks towards 2,  $\Delta\lambda_{min}$  tends towards 0, overshooting slightly. We also see that the difference  $\Delta\lambda_{min}$  is almost always positive, with few exceptions, and even the layers that do not overshoot form a kind of “funnel shape pointing towards the critical point (2,0). In (c), (ViT,) we also see the same general relationship between  $\alpha$  and  $\Delta\lambda_{min}$  across layers of several ViT models. Observe that ViT models do not have convolutional layers, and in spite of this, the overall pattern is similar. In (d), (DenseNet,) we see a similar overall trend as in (b), except that  $\Delta\lambda_{min}$  tends to decrease sooner, but there are also more layers with  $\alpha < 2$  and  $\Delta\lambda_{min}$  above 0.

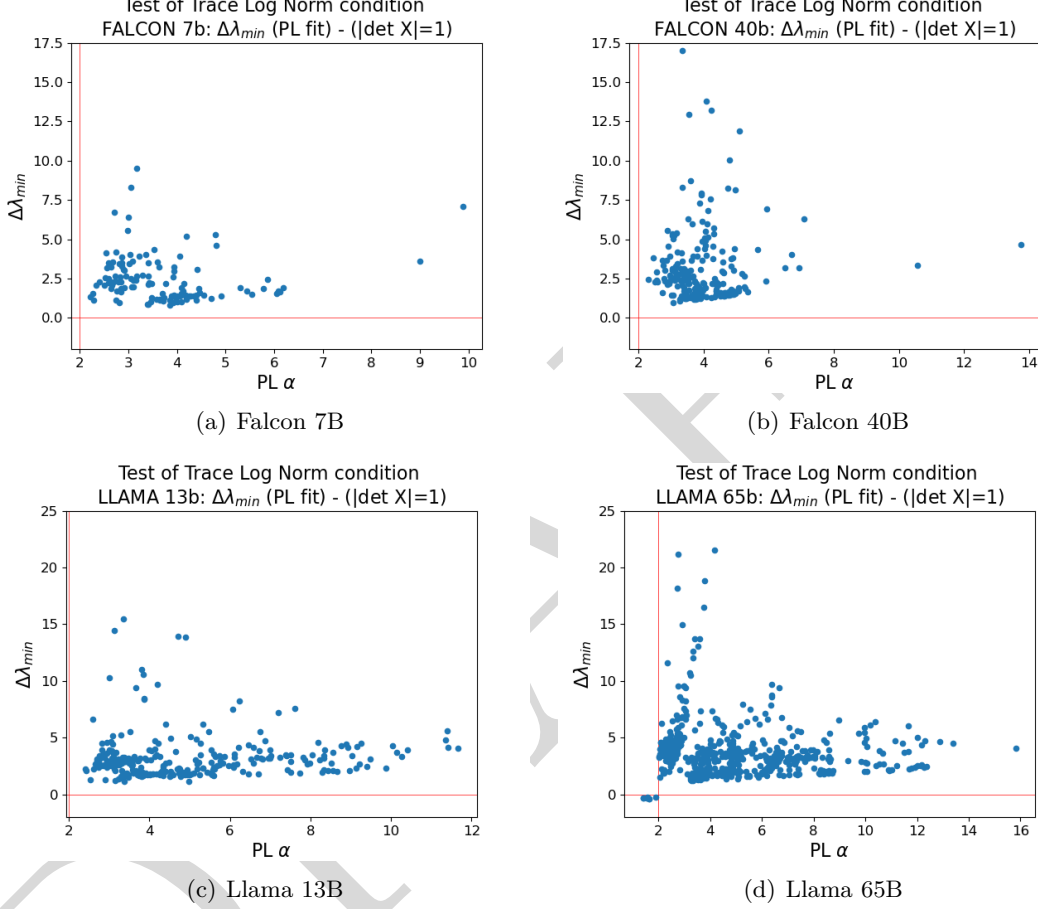


Figure 23: Difference between the two  $\lambda_{min}$  estimates,  $\Delta\lambda_{min} = \lambda_{min}^{PL} - \lambda_{min}^{|det X|=1}$ , as a function of  $\alpha$ , for all linear layers in the FALCON[125](a-b) and LLAMA [126](c-d) language models for varying numbers of parameters. As in Figure 22, we see that in recent Large Language Models,  $\Delta\lambda_{min}$  remains positive, except where  $\alpha < 2$  (d). Otherwise, a “funnel shape can still be seen leading towards the critical point (2,0) as in Figures 22(b) and 22(c). Observe that the x- and y-axes are different between sub-figures due to the differences in scale of each model.

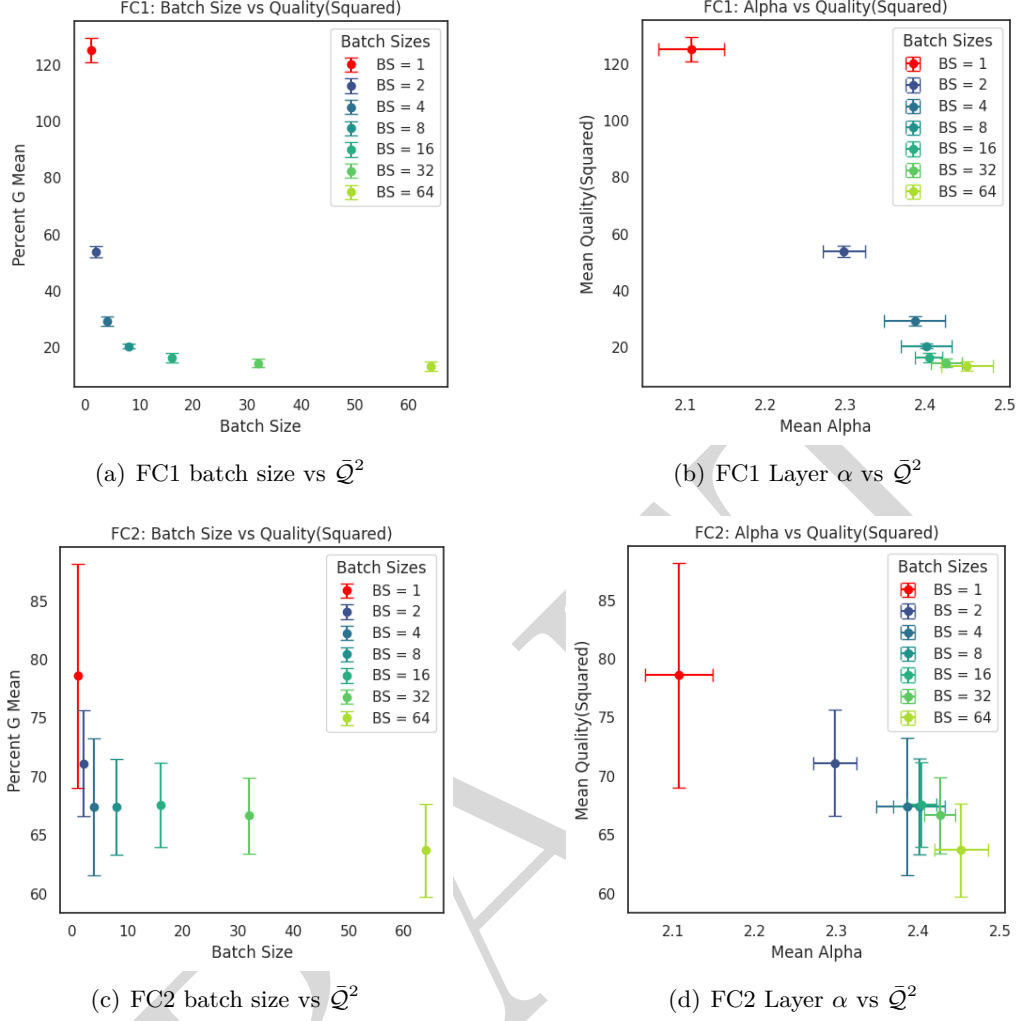


Figure 24: Evaluation of the computational R-transform Layer Quality-Squared metric  $\bar{Q}^2$  on the fully trained MLP3 model(s) for different batch sizes.

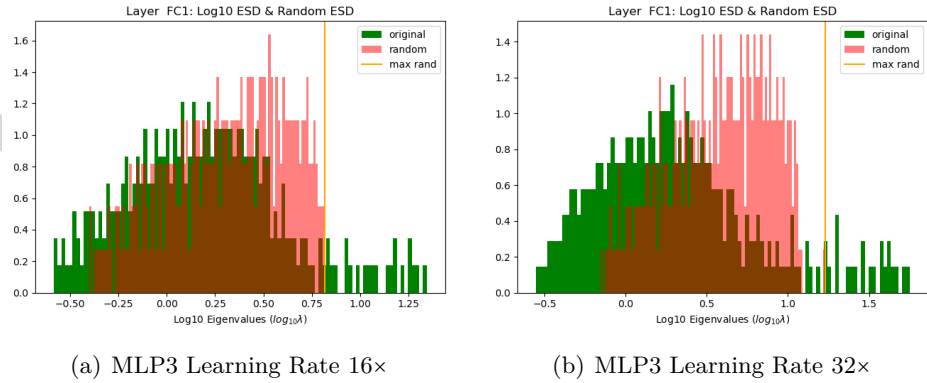


Figure 25: ESD plots for learning rate  $lr = 16\times$  and  $lr = 32\times$  normal, shown on Log-Lin scale, as computed using the `WeightWatcher` tool, for the FC1 weight matrix  $\mathbf{W}$  (green) and an element-wise randomized  $\text{rand}(\mathbf{W})$  (red). This provides an example of inducing a Correlation Trap in the MLP3 model, simply by increasing the learning rate used during model training. See Section 3.3.1.

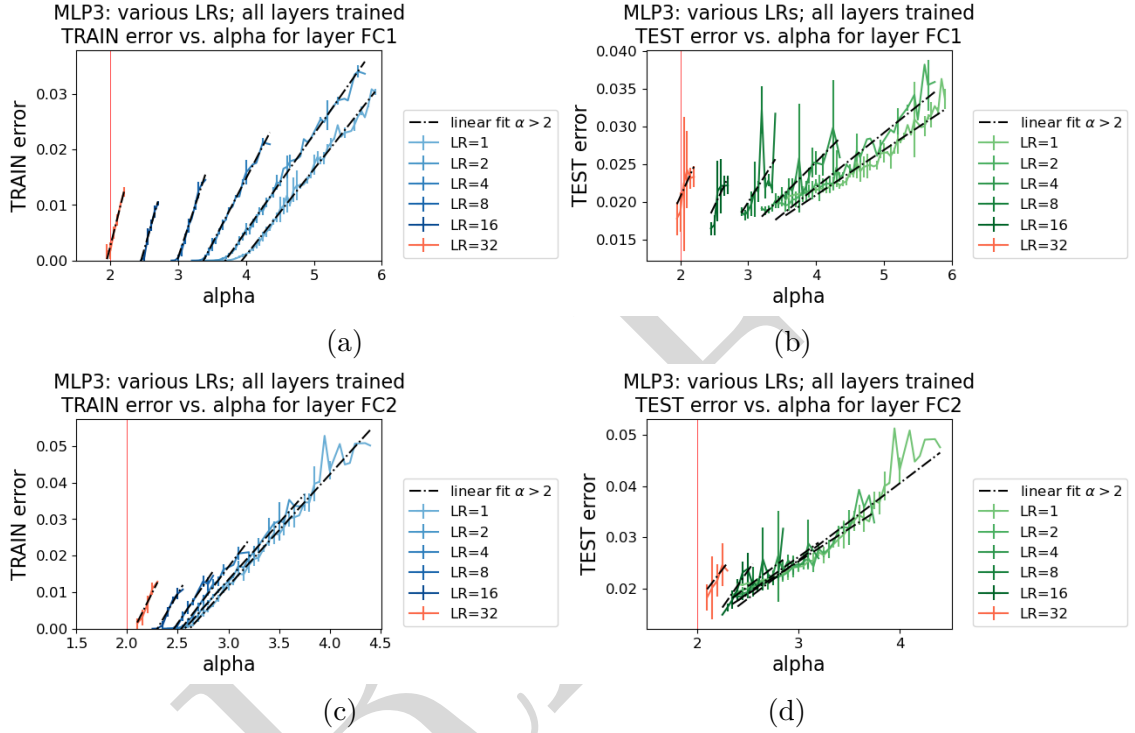


Figure 26: Train (a, c) and test (b, d) accuracy as a function of  $\alpha_{FC1}$  (a, b) and  $\alpha_{FC2}$  (c, d) when **all layers are trained**. Red vertical lines show the critical value of  $\alpha = 2$ , and dashed black lines show linear fits of error, using only points where  $\alpha > 2$  and train error  $> 0.001$ . For FC1 (a, b), we can see that each learning rate produces a different trajectory of train error (a) and test error (b) as a function of  $\alpha_{FC1}$ , showing that even though FC1 dominates overall, (Table 10,) FC2 still plays a modulating role. (Cf. Figure 27 where there is only one trajectory.) In (c, d) we can see that  $\alpha_{FC2}$  never goes below 2. As in (a, b), each learning rate produces a different trajectory, though there is greater overlap for lower learning rates. See discussion in Section 6.6.1.

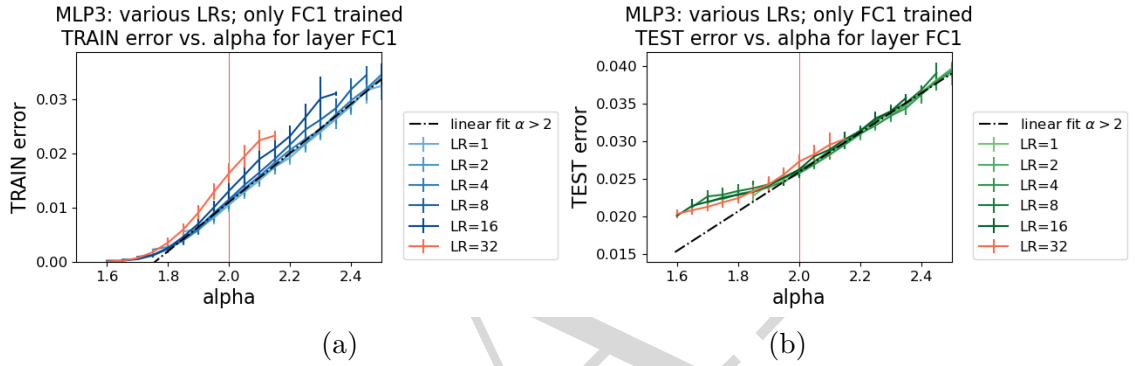
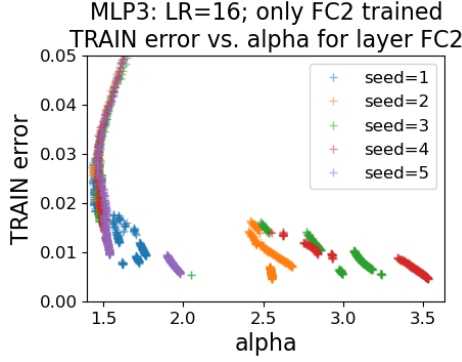
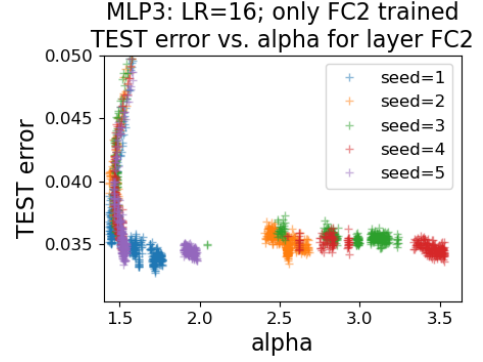


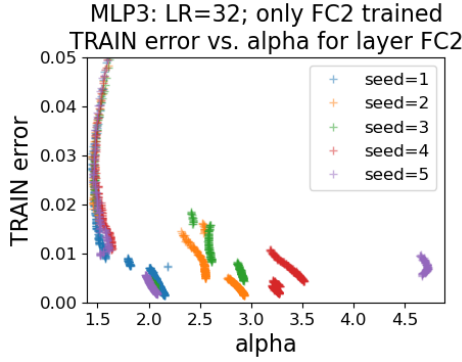
Figure 27: Train and test accuracy as a function of  $\alpha_{FC1}$  when only FC1 is trained (a, b). Red vertical lines show the critical value of  $\alpha_{FC1} = 2$ , and dashed black lines show linear fits of error, using only points where  $\alpha_{FC1} > 2$ . In contrast with Figure 26, when only FC1 is trained, we can see that no matter the learning rate, there is only one trajectory, for both train error (a) and test error (b). Hence, for visibility, only one linear fit, using all learning rates pooled, is shown. Crucially, we can see in (b) that as  $\alpha_{FC1}$  passes below 2, the *test error* trajectory changes, for all learning rates, even as the *train error* trajectory does not, until it reaches  $\sim 0$ . This suggests that even though test accuracy can still decrease when  $\alpha_{FC1} < 2$ , it does so at a decreased rate relative to  $\alpha_{FC1}$ . See discussion in Section 6.6.2.



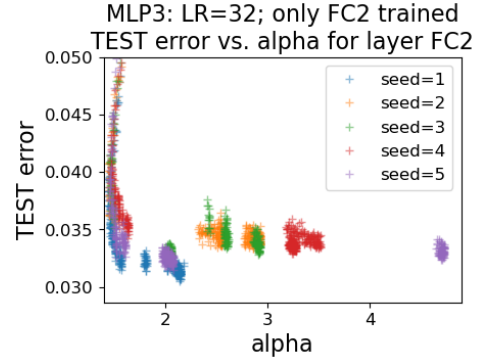
(a)



(b)



(c)



(d)

Figure 28: Train error (a, c) and test error (b, d) as a function of  $\alpha_{FC2}$  when all other layers are frozen, for the two largest learning rates,  $lr = 16\times$ , (a, b) and  $lr = 32\times$  (c, d). Cf. Figure 26, wherein all layers were trained. Due to the markedly different behavior of each random seed, they cannot be plotted as means and error bars, and are instead shown separately. The path taken by all seeds up to  $\alpha_{FC2} = 1.5$  has a slight curvature characteristic of a hysteresis-like behavior. Observe also that the fragmenting into separate paths, due to the breakdown of the PL tail, coincides roughly with each seeds path reaching its minimum test error. The y-axis is scaled differently for train and test error to make variation more visible. See discussion in Section 6.6.3.



## 7 Conclusion and Future Directions

In this work, we have introduced **SETOL**, a *Semi-Empirical Theory of (Deep) Learning* that unifies concepts from Statistical Mechanics (**StatMech**), Heavy-Tailed (HT) Random Matrix Theory (RMT), and quantum-chemistry-inspired approaches to strongly correlated systems [53, 54, 55]. **SETOL** aims to provide a solid theoretical foundation for the Heavy-Tailed Self-Regularization (HTSR) phenomenology, including the widely used **Alpha** and **AlphaHat** HT Power Law (PL) Layer Quality metrics, which are implemented in the open-source **WeightWatcher** toolkit. Specifically, **SETOL** reformulates the Neural Network (NN) learning problem for a single layer as a matrix generalization of the Student-Teacher (ST) model for Perceptron learning, where the Teacher is now taken as empirical input, and the result is in Annealed Approximation (AA) at high temperatures (high-T). This reformulation results in a Free Energy (i.e., Generating Function  $\beta\Gamma_{Q^2}^{IZ}$ ) expressed as an integral over random Student correlation matrices, commonly referred to as the Harish-Chandra–Itzykson–Zuber (HCIZ) integral. To evaluate this integral, we recast the solution using a technique derived from first principles, analogous to a taking single step of the Wilson Exact Renormalization Group (ERG) theory [56, 57]. Leveraging more recent results [83, 84], we express the Layer Quality as a sum of integrated matrix-cumulants from RMT (i.e., R-transforms). Finally, we conduct both direct and observational experiments to validate key assumptions of the **SETOL** framework and empirically connect it to the HTSR theory.

### Key Contributions and Observations.

- A. *Rigor for the HTSR Phenomenology.* **SETOL** explains *why* power-law (PL) exponents in the layer spectral densities (e.g. **Alpha** and **AlphaHat**) act as robust diagnostics of generalization, even in large, complex architectures without access to training or test data. Our analysis ties these Heavy-Tailed ESDs to a Scale-Invariant Volume Preserving Transformation associated with an *Effective* Free Energy, and suggesting (in analogy with traditional **StatMech** phases in learning theory) that the HTSR condition  $\alpha \approx 2$  marks a phase boundary between optimal generalization and overfitting.
- B. *Matrix-Generalized Student-Teacher (ST) Model.* **SETOL** is formulated as Semi-Empirical matrix generalization of the classical (vector-based) ST perceptron learning, taking the Teacher now as empirical input, and incorporating  $N \times M$  layer weight matrices,  $\mathbf{w} \rightarrow \mathbf{W}$ . Key to this generalization is isolating the top eigenvalue/eigenvector directions—called the *Effective Correlation Space* (**ECS**)—before evaluating the resulting partition function (or HCIZ integral). The ECS contains the HTSR PL tail, validating that the tail captures the dominant layer generalizing components.
- C. *ERG Condition & Alpha = 2.* A remarkable empirical observation, predicted by **SETOL**, is that layers near *ideal* training also satisfy a  $\prod \tilde{\lambda}_i \approx 1$  in their tail eigenvalues (i.e.,  $|\det X| = 1$ ); equivalently,  $\sum \ln \tilde{\lambda}_i = \ln \prod \tilde{\lambda}_i \approx 0$ . We call this the **ERG** condition (i.e, the *detX* option in **WeightWatcher**). Empirically, this condition appears when the HTSR **Alpha**  $\approx 2$ . **SETOL** thereby *unifies* two previously separate heuristics for “optimal” or so-called Ideal behavior.
- D. *Empirical Validation of SETOL.* To validate the **ERG** and the **ECS** conditions, we trained small (3-layer) Multi-Layer Perceptron (MLP3) on MNIST and under varying batch sizes and learning rates. Using this, we verified that when the HTSR  $\alpha \approx 2$  the **SETOL** **ERG** condition also (usually) holds, and that one can reproduce the training accuracy by retaining only the **ECS**. This is further confirmed by using the **WeightWatcher** tool to examine the **Alpha** and **DetX** metrics common, open-source CV and NLP models, including modern LLMs (ResNets, DenseNets, ViTs, and LLMs like LLaMA and Falcon).

E. *Correlation Traps & OverFitting.* We observe that when layer ESDs with  $\alpha < 2$ , they exhibit behavior interpreted as *over-regularization* and/or *overfitting*. For example, we observe what we call *Correlation Traps*, large rank-one perturbations in the (randomized) layer weight matrix  $\mathbf{W}$  that can be induced by training with excessively small batch sizes (bs=1) and/or large learning rates, and are associated with degraded test accuracy, and which cause the HTSR to drop to  $\alpha < 2$ . These results are consistent with other results, applying HTSR theory to understand Grokking[108].

Additionally, we can induce overfitting by freezing all but one layer and then training, which causes the layer  $\alpha < 2$ . By training in the underparameterized regime, we observe path-dependent, “glassy” behavior.

F. *OverParameterized and UnderParameterized regimes.* These above results indicate that the HTSR and SETOL approaches can be applied effectively in the overparameterized regime, even in conditions beyond the apparent range of validity of the theory ( $\alpha \gg 2$ ). In the underparameterized regime, they are less effective. It is noted that modern transformers like LLMs may appear to be underparameterized, but the multiplicative nature of their interactions suggests they are overparameterized. [128], making HTSR and SETOL very applicable for such AI models.

G. *Connection to Semi-Empirical Methods.* Conceptually, SETOL parallels well-known *Semi-Empirical* methods in quantum chemistry [53, 54, 55], wherein complicated many-body Hamiltonians are approximated by effective theories, but fitted or validated using empirical data. By retaining only the largest spectral modes (ECS) and imposing the ERG condition, we can describe crucial low-rank correlations while discarding less relevant interactions, much like in Freed–Martin Effective Hamiltonian and/or Wilson’s Exact Renormalization Group (ERG) approach [51, 94, 53, 54, 52, 55, 57].

**ERG Analogy: A One-Step View.** From a Renormalization Group perspective, restricting to the measure on the partition function to the ECS is akin to performing a *single step* of the Wilson Exact Renormalization Group (ERG). In doing this, we are discarding bulk “uninteresting” degrees of freedom in favor of the strongly correlated HT *long-ranged* modes. This leads to an effective model with fewer degrees of freedom but *renormalized* interactions—interactions that are dominated by the largest eigenvalues. This analogy with ERG theory suggests that the HTSR phenomenology, where  $\alpha \in [2, 6]$  in the Fat-Tailed Universality Class, is essentially describing a near-critical phase when  $\alpha \approx 2$  and satisfies  $\text{Tr}[\ln \tilde{\lambda}] = \ln \prod \tilde{\lambda}_i \approx 0$  in its ECS. Departing from this point ( $\alpha < 2$ ) leads to suboptimal results, consistent with the multi-phase pictures in StatMech spin glass theories of learning [8, 6, 4, 5].

**Toward Understanding “Why Deep Learning Works.”** A key question in deep learning theory is why large neural networks achieve strong generalization despite operating in highly non-convex optimization landscapes. From the perspective of ERG theory, this phenomenon can be partially understood through the concentration of generalization-relevant components. Specifically, models trained in regimes exhibiting *Power-Law (PL)* correlations lead to the emergence of effective low-dimensional descriptions, where irrelevant modes are suppressed. The **WeightWatcher Alpha** metric quantitatively captures this concentration by characterizing how the optimization landscape stabilizes near criticality, with  $\alpha \approx 2$  signaling optimal generalization.

**Student-Teacher Knowledge Distillation.** SETOL also provides an explanation of why Student-Teacher distillation works so well. When training a Student DNN  $S$  to emulate a larger Teacher

$T$ , the Student inherits the inductive biases and generalization behavior of Teacher, which SETOL explains is concentrated in  $T$  into smaller (lower rank) layer weight matrices. Thus, the Student converges to a similar region of the optimization landscape, shaped by the same spectral and statistical constraints that govern the Teacher, allowing for a smaller model to effectively mimic, if not reproduce, the Teacher’s outputs.

**A Novel Way to Characterize Generalization.** Many results that use the AA / High-Temperature limit effectively state that “with enough data and a wide enough NN, one can learn anything”. But how much is “enough”? SETOL takes this one step further by giving useful empirical measures that converge to the same Ideal, whose progress can be precisely tracked in finite settings. Our experimental results show that this occurs both in a simple model, as well as in large production models. These measures strongly indicate the point at which further learning in a particular layer will be counterproductive.

**Relation to Levy Spin Glasses and Heavy-Tailed Random Matrix Models.** One long-standing puzzle is why large NNs avoid the worst of highly non-convex optimization, despite nominal exponential degeneracies. SETOL offers a partial explanation: if the trained model has *Levy-like* or VHT PL correlations, then typical spin-glass degeneracies can be lifted, leaving the layer in a finite number of near-critical minima. In analogy with older work on *Levy Spin Glasses*[40], it is proposed **WeightWatcher Alpha** metric effectively measures how *rugged yet stable* the effective energy landscape is for each layer, with  $\alpha \approx 2$  signifying a sweet spot of Ideal generalization.

## 7.1 Future Directions

**1. Multi-Layer ERG and Layer Interactions.** While SETOL is formulated per-layer, modern DNNs stack many layers, each potentially with different  $\alpha$ . An improved approach would treat layer-layer interactions (relax the IFA). It is possible that certain layers (e.g. final fully-connected heads in LLMs) exhibit  $\alpha$  far from 2, while others converge near 2—raising questions about how best to address or combine them.

**2.. Practical Diagnostics and Fine-Tuning.** The open-source **WeightWatcher** tool has already seen success diagnosing layer quality. Integrating SETOL’s ERG condition may refine this further, helping users identify correlation traps or “under-exploited” layers. There is also strong potential for using **Alpha** and ERG-based signals during training or fine-tuning in the training of very large LLMs: e.g. automatically adapting learning rates to push each layer closer to  $\alpha = 2$ [27], for fine-tuning models with significantly less memory[129], for compressing large LLMs[30], and other practical applications.

**3. Correlation Traps and Meta-Stable States.** Although our experiments show how small batch sizes or large learning rates can induce correlation traps, a quantitative theory of *where and why* traps occur remains open. Clarifying these states could enable *trap-avoidance* strategies, e.g. partial re-initialization or specialized regularizers that favor lower-rank updates in the ECS. In large-language-model (LLM) contexts, correlation traps might manifest as *hallucinations* or *mode collapse*, motivating deeper analysis.

**4. Analyzing the Layer Null Space.** One critical but often overlooked factor is the potential null space within model layers, which can emerge during overfitting. This null space represents parameter directions that fail to contribute meaningfully to generalization but instead

2874 encode redundant or overly specific patterns tied to the training data which might be ignored  
 2875 or forgotten. Future work should examine if and when NN layers have components in their null  
 2876 space, which contribute significantly to the performance of the model.

2877 **5. Layer-Layer Cross-Terms.** SETOL is a single layer theory, however, as noted in Sec-  
 2878 tion 5.1, it would be desirable to extend the theory to including layer-layer cross terms. While  
 2879 we don’t have an exact expression for this, we can propose a phenomenological guess that the  
 2880 leading order term would be the integrated R-transform, defined for the overlap between nearest-  
 2881 neighbor weight matrices (i.e.,  $\mathbf{W}_1, \mathbf{W}_2$ ) that can be aligned along a common axis. This term  
 2882 would take the form  $\mathbb{G}_{\mathbf{R}_{1,2}}(\lambda_{1,2})$  where  $\mathbf{R}_{1,2} \sim \mathbf{W}_1^T \mathbf{W}_2$  and  $\lambda_{1,2}$  is an eigenvalue of  $\mathbf{R}_{1,2}$ . Note that  
 2883 the open-source **WeightWatcher** tool can identify and compute the intra-layer interactions.[67]

2884 **Concluding Remarks.** SETOL as a Semi-Empirical theory merges first-principles methods from  
 2885 **StatMech** and RMT with empirical insights from HTSR and the open-source **WeightWatcher** tool.  
 2886 It clarifies *how* Heavy-Tailed layer weight matrices can emerge from training on realistic data,  
 2887 and *why* their spectral exponents so reliably predict generalization quality without peeking at  
 2888 training/test sets. In so doing, **SETOL** not only offers new insights into the “*why does it work*”  
 2889 question of deep learning but also suggests a roadmap for improving DNN models by focusing  
 2890 attention on that near-critical subspace of their largest eigenvalues. We are optimistic that  
 2891 future developments along these lines—extending the single-step Wilson Exact Renormalization  
 2892 Group analogy, understanding layer-layer interactions expansions, and systematically diagnosing  
 2893 correlation traps, and developing better large-scale training methods—will yield more robust,  
 2894 data-free metrics for training, fine-tuning, and compressing next-generation neural networks.

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## A Appendix

### A.1 Data Vectors, Weight Matrices, and Other Symbols

See Table 11 for a summary of various vectors and matrices, including their dimensions; see Table 12 for a summary of various symbols used throughout the text; and see Table 13 for a summary of types of “Energies” used throughout the text.

Number of NN Layers	index $L$	$N_L$
Number of Data Examples	index $\mu$	$n$
Number of (input) Features	index $i, j$	$m$
Actual Data (Matrix)	$D$	$n \times m$
Model Data (Matrix)	$\mathcal{D}$	$n \times m$
Teacher Perceptron Weight Vector	$\mathbf{t}$	$m$
Student Perceptron Weight Vector	$\mathbf{s}$	$m$
Actual Input Data Vector	$\mathbf{x}_\mu$	$N_f \times 1$
Gaussian model of Input Data Vector	$\boldsymbol{\xi}_\mu$	$N_f \times 1$
Actual Input Data Label	$y_\mu$	$+1   -1$
Model Input Data Label	$\hat{y}_\mu$	$+1   -1$
General Weight Matrix	$\mathbf{W}$	$N \times M$
General Correlation Matrix	$\mathbf{X} = \frac{1}{N} \mathbf{W}^\top \mathbf{W}$	$M \times M$
Input Layer Weight Matrix	$\mathbf{W}_1$	$N \times M$
Hidden Layer Weight Matrix	$\mathbf{W}_2$	$N \times M$
Output Layer Weight Matrix	$\mathbf{W}_3$	$M \times 2$
Teacher Weight Matrix	$\mathbf{T}$	$N \times M$
Student Weight Matrix	$\mathbf{S}$	$N \times M$
Student-Teacher Overlap Matrix	$\mathbf{R} = \frac{1}{N} \mathbf{S}^\top \mathbf{T}$	$M \times M$
Inner Student Correlation Matrix	$\mathbf{A}_M = \frac{1}{N} \mathbf{S}^\top \mathbf{S}$	$M \times M$
Outer Student Correlation Matrix	$\mathbf{A}_N = \frac{1}{N} \mathbf{S} \mathbf{S}^\top$	$N \times N$
Inner ECS Student Correlation Matrix	$\tilde{\mathbf{A}}_M$	$M \times M$
Outer ECS Student Correlation Matrix	$\tilde{\mathbf{A}}_N$	$N \times N$
ECS Teacher Correlation Matrix	$\tilde{\mathbf{X}}$	$M \times M$

Table 11: Summary of various vectors and matrices, including their dimensions.



Perceptron Student-Teacher (ST) Overlap	$R = \mathbf{s}^\top \mathbf{t} = \sum_i s_i t_i$
Student-Teacher (ST) Overlap Operator	$\mathbf{R} = \frac{1}{N} \mathbf{S}^\top \mathbf{T}$
Matrix Generalized ST Overlap	$\frac{1}{N^2} \text{Tr} [\mathbf{R}^\top \mathbf{R}]$
Student-Teacher Self-Overlap	$\eta(\boldsymbol{\xi}^n) = \mathbf{y}_T^\top \mathbf{y}_S$
$\ell_2$ -Energy or $\ell_2$ -Error	$E_{\ell_2}(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi})$
$\ell_2$ -Energy Operator Form	$E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) := \sum_{\boldsymbol{\xi}} E_{\ell_2}(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi})$
$\ell_2$ -Energy Matrix Operator Form	$E_{\ell_2}^n(\mathbf{S}, \mathbf{T}) := N(\mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T})$
Annealed Error Potential	$\epsilon(R) = \epsilon(S, T) = \langle E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}^n) \rangle_{\boldsymbol{\xi}^n}$
Linear Perceptron $\epsilon(R)$ at high-T, large- $N$	$\epsilon(R) = 1 - R$
Annealed Approximation (AA)	$\langle \ln Z \rangle_{\boldsymbol{\xi}^n} \approx \ln \langle Z \rangle_{\boldsymbol{\xi}^n}$
Annealed Hamiltonian	$H^{an}(\mathbf{w})$
Annealed Hamiltonian at high-T	$H_{hT}^{an}(\mathbf{w}) = \epsilon(\mathbf{w})$
Average Student-Teacher Generalization Error	$\bar{\mathcal{E}}_{gen}^{ST} = \langle \epsilon(R) \rangle_{\mathbf{s}}^\beta$
Average Student-Teacher Generalization Accuracy	$1 - \bar{\mathcal{E}}_{gen}^{ST} = \langle \eta(R) \rangle_{\mathbf{s}}^\beta$
Matrix Layer Quality-Squared	$\bar{\mathcal{Q}}^2 = \langle \mathbf{R}^\top \mathbf{R} \rangle_{\mathbf{S}}^\beta$
Equivalent Notation for Averages	$\langle \cdots \rangle_A = \int \cdots d\mu(\mathbf{A}) = \mathbb{E}_{\mathbf{A}}[\cdots]$
Projection Operator onto ECS	$\mathbf{P}^{ecs} := \sum  \tilde{\lambda}_i\rangle \langle \tilde{\lambda}_i , i = 1 \cdots \tilde{M}$
Average over ECS Student Correlation Matrices	$\langle \cdots \rangle_{\tilde{\mathbf{A}}}^\beta = \int \cdots d\mu(\tilde{\mathbf{A}}) = \mathbb{E}_{\tilde{\mathbf{A}}}[\cdots]$
ERG Trace-Log-Determinant Relation	$\text{Tr} [\ln \mathbf{A}] = \ln \det \mathbf{A}$
Effective Correlation Measure Transform	$d\mu(\mathbf{S}) \rightarrow d\mu(\tilde{\mathbf{A}})$
HCIZ Integral (Tanaka's Notation)	$\mathbb{E}_{\tilde{\mathbf{A}}} [\exp(n\beta \text{Tr} [\mathbf{T}^\top \mathbf{A} \mathbf{T}])]$
HCIZ Integral (Large- $\mathcal{N}$ in $N$ explicit)	$\langle \exp(n\beta N \text{Tr} [\frac{1}{N} \mathbf{T}^\top \tilde{\mathbf{A}}_N \mathbf{T}]) \rangle_{\tilde{\mathbf{A}}}$
Layer Quality-Squared Generating Function	$\beta \mathbf{T}_{\bar{\mathcal{Q}}^2, N \gg 1}^{IZ} := n\beta \sum_{\mu=1}^{\tilde{M}} \int_{\tilde{\lambda}_{min}}^{\tilde{\lambda}_{\mu}} dz R(z)$
Norm Generating Function	$G_A(\gamma) = \int_{\tilde{\lambda}_{min}}^{\tilde{\lambda}} R_A(z) dz$
Eigenvalue for $\mathbf{X} = \frac{1}{N} \mathbf{W}^\top \mathbf{W}$	$\lambda$ or $\lambda_i$ for $i = 1 \cdots M$
Power Law ESD Tail for $\mathbf{X}$	$\rho_{tail}(\lambda) \sim \lambda^{-\alpha}$
Effective Correlation Space ESD Tail for $\mathbf{X}$	$\rho_{tail}^{ECS}(\tilde{\lambda}), \text{Tr} [\ln \prod_{j=1}^{\tilde{M}} \tilde{\lambda}_j] = 0$
Schatten Norm	$\ \mathbf{X}\ _\alpha^\alpha = \sum_j \lambda_j^\alpha$
ECS Tail Norm	$\frac{1}{\tilde{M}} \sum_i^{\tilde{M}} \tilde{\lambda}_i, \tilde{\lambda}_i \in \rho_{tail}^{ECS}(\lambda)$
Spectral Norm	$\ \mathbf{X}\ _\infty = \lambda_{max}$
WeightWatcher Start of PL Tail	$\lambda_{min}^{PL} = \lambda_{min}$
Start of ECS Tail	$\lambda_{min}^{ECS} = \lambda_{min}^{ det X =1}$
ECS-PL Gap between start of tails	$\Delta \lambda_{min} := \lambda_{min}^{ECS} - \lambda_{min}^{ det X =1}$
WeightWatcher Alpha (layer) quality metric	$\alpha$
WeightWatcher AlphaHat (layer) quality metric	$\hat{\alpha} = \alpha \log_{10}(\lambda_{max})$

Table 12: Summary of various various symbols used throughout the text.

Explanation	Examples	Refs
<b>Energy Landscape or NN Output function</b> The output of the NN given a single input data point.	$E_{NN}^{out}$	Sec. 2.1 1,77,4.3.1,100
<b>Energy or Student-Teacher (ST) Error</b> The squared between the output of a Student NN and its prescribed Teacher label $y_\mu^T$ for a single data point And as the total error for a sample of $n$ data points Or between the outputs of the Student and the Teacher NNs.	$E_{\mathcal{L}}, E_{\mathcal{L}}^n$ $E_{\mathcal{L}}(\xi_\mu) := (y_\mu^T - E_S^{out}(\xi_\mu))^2$ $E_{\mathcal{L}}^n = \sum_{\mu=1}^n E_{\mathcal{L}}(\xi_\mu)$ $E_{\mathcal{L}}^n := \sum_{\mu=1}^n (E_S^{out}(\xi_\mu) - E_T^{out}(\xi_\mu))^2$	Sec. 4, A.2 19 22 86,101,183
<b>Annealed Hamiltonian (and Potentials)</b> The Annealed Error Potential (for the Error) is defined as: The Annealed Hamiltonian (for the Error): At high-T, the relation between $H_{hT}^{an}$ and $\epsilon(R)$ is The full ST model Hamiltonian: At high-T, the ST model Hamiltonian is: The per-parameter ST model Hamiltonian: At high-T, the matrix-generalized ST model Hamiltonian is: The Layer Quality-Squared Hamiltonian (for the Accuracy):	$H^{an}(\mathcal{E}(R), \epsilon(R))$ $\epsilon(R) = \frac{1}{n} \mathcal{E}(R) = \langle E_{\mathcal{L}}^n \rangle_{\xi^n}$ $\beta H^{an} := \frac{1}{n} \ln \langle e^{-\beta E_{\mathcal{L}}^n} \rangle_{\xi^n}$ $H_{hT}^{an}(R) := \epsilon(R)$ $\beta H^{an}(\beta, R) := \frac{1}{2} \ln[1 + 2\beta(1 - R)]$ $\beta H_{hT}^{an}(R) := \beta(1 - R)$ $\beta h^{an}(\mathbf{R}) := \frac{1}{2} \ln[1 + \frac{2\beta N}{M} \text{Tr}[\mathbf{I}_M - \mathbf{R}]]$ $H_{hT}^{an}(\mathbf{R}) := N(\mathbf{I}_M - \mathbf{R})$ $\mathbf{H}_{\bar{Q}^2} := \mathbf{R}^\top \mathbf{R}$	Sec. 4.2.4, A.2 97 43, 168 49 175 97, 176 200 206 16, 218
<b>Different Average Model Errors</b> Empirical Training, Teacher, and Test Errors Empirical Generalization Gap Student-Teacher Training and Generalization Errors Neural Network (MLP) Training and Generalization Errors, the (abstract) matrix generalization of ST error	$\bar{\mathcal{E}}$ $\bar{\mathcal{E}}_{train}^{emp}, \bar{\mathcal{E}}^T \approx \bar{\mathcal{E}}_{gen}^{emp}$ $\bar{\mathcal{E}}_{gap}^{emp} := \bar{\mathcal{E}}_{train}^{emp} - \bar{\mathcal{E}}_{gen}^{emp}$ $\bar{\mathcal{E}}_{train}^{ST}, \bar{\mathcal{E}}_{gen}^{ST}$ $\bar{\mathcal{E}}_{train}^{NN}, \bar{\mathcal{E}}_{gen}^{NN}$	Sec. 4.2.5 78,79,83 84 171,174
<b>Average Training and/or Generalization Error</b> In the AA and at High-T, these are the same, and are just the Thermal Average of $\epsilon(R)$ For the ST model, we always assume AA and High-T Likewise, when generalizing $\bar{\mathcal{E}}_{gen}^{ST}$ to matrices,	$\bar{\mathcal{E}}_{train}, \bar{\mathcal{E}}_{gen}$ $\bar{\mathcal{E}}_{train}^{an, hT} = \bar{\mathcal{E}}_{gen}^{an, hT} = \langle \epsilon(R) \rangle_{\mathbf{s}}^\beta$ $\bar{\mathcal{E}}_{gen}^{ST} = \bar{\mathcal{E}}_{gen}^{an, hT}$ $\bar{\mathcal{E}}_{gen}^{ST} \rightarrow \bar{\mathcal{E}}_{gen}^{NN} = \bar{\mathcal{E}}_{gen}^{an, hT}$	Sec. 4.2.5 56,54
<b>Layer Qualities</b> For the ST Perceptron, $\bar{Q}^{ST}$ is the generalization accuracy in terms of the Self-Overlap $\eta(R)$ In the AA, and at high-T, $\langle \epsilon(R) \rangle_{\mathbf{s}}^\beta = 1 - R$ For an MLP / NN, we approximate the total accuracy as a product of layer qualities $\bar{Q}$ (in the AA, at high-T) For a matrix, the Layer Quality-Squared $\bar{Q}^2$ We approximate $\bar{Q}$ using the quality squared	$\bar{Q}, \bar{Q}^2$ $\bar{Q}^{ST} := 1 - \bar{\mathcal{E}}_{gen}^{ST} = 1 - \langle \epsilon(R) \rangle_{\mathbf{s}}^\beta$ $\bar{Q}^{ST} := \langle \eta(R) \rangle_{\mathbf{s}}^\beta$ $\bar{Q}^{ST} := 1 - \bar{\mathcal{E}}_{gen}^{an, ht} = \langle R \rangle_{\mathbf{s}}^\beta$ $\bar{Q}^{NN} := \prod \bar{Q}_L^{NN}$ $\bar{Q}^2 := \langle \mathbf{R}^\top \mathbf{R} \rangle_{\mathbf{s}}^\beta$ $\bar{Q} := \sqrt{\bar{Q}^2} \approx Q_L^{NN}$	Sec. 5.2.1, A.3 99 7 110 9,111

Table 13: Summary of types of “Energies,” with simplified examples of the notation, and references to definitions.

## A.2 Summary of the Statistical Mechanics of Generalization (SMOG)

In this section, we derive the Annealed Hamiltonian for two variants of the ST model, in the high-T limit: in Appendix A.2.1, we derive an expression for  $H^{an}(R)$  for the ST Perceptron model, when the students and teachers are modeled as  $N$ -vectors  $\mathbf{w}$  (as in [8]); and in Appendix A.2.2, we derive an expression for  $H^{an}(\mathbf{R})$  for Matrix-Generalized case, i.e., when the students and teachers are modeled as  $N \times M$  matrices  $\mathbf{W}$  (as our SETOL requires). From these, we will obtain expressions for the Average ST Model Generalization Accuracy  $\bar{\mathcal{E}}_{gen}^{ST}$  and the Average NN Model Generalization Accuracy  $\bar{\mathcal{E}}_{gen}^{NN}$ , as well as for the corresponding data-averaged errors. Although the functional form for these quantities will be the same for the vector case and the matrix case, there are several important differences in the derivation of  $H^{an}(\mathbf{R})$ , most notably having to do with a normalization for the weight matrix.

### A.2.1 Annealed Hamiltonian $H^{an}(R)$ when Student and Teachers are Vectors

In this section, we derive an expression for the Annealed Hamiltonian  $H^{an}(R)$ , in the AA and the high-T approximation, when student and teachers are modeled as  $N$ -vectors. From this, we obtain an expression for the data-averaged ST error  $\epsilon(R)$ , which is the same as the expression given in Eqn. 97.

The procedure starts by computing the associated quenched average of the Free Energy, defined for the model error as

$$\begin{aligned} \langle -\beta F \rangle_{\xi^n} &:= \langle \ln Z \rangle_{\xi^n} \\ &= \left\langle \ln \int d\mu(\mathbf{s}) e^{-\beta E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \xi^n)} \right\rangle_{\xi^n} \\ &= \frac{1}{N} \int d\mu(\xi^n) \ln \int d\mu(\mathbf{s}) e^{-\beta E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \xi^n)}, \end{aligned} \quad (165)$$

where  $d\mu(\xi^n) := \prod_{i=1}^N d\xi_i P(\xi^n)$  and where the data-dependent ST error,  $E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \xi^n)$ , is defined in Eqn. 86, with an  $\mathcal{L} = \ell_2$  loss.<sup>47</sup> If we apply the AA (see Eqn. 40 and Eqn. 41) to Eqn. 165, then we obtain

$$\langle -\beta F \rangle_{\xi^n} \simeq \ln \frac{1}{n} \int d\mu(\xi^n) \int d\mu(\mathbf{s}) e^{-\beta E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \xi^n)}. \quad (166)$$

Notice that we have interchanged the logarithm ( $\ln$ ) and the data average (the “disorder average”)  $\langle \cdots \rangle_{\xi^n}$  over the data; this is the essence of the AA, as it lets the disorder fluctuate rather than forcing the system to be quenched to the data. We will now switch the order of integration in Eqn. 166, giving

$$\langle -\beta F \rangle_{\xi^n} \simeq \ln \int d\mu(\mathbf{s}) \frac{1}{n} \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \xi^n)}. \quad (167)$$

We now recall the definition of the Annealed Hamiltonian,  $H^{an}(R)$  (see Eqn. 43 in Section 4.2, which is analogous to Eqn. (2.31) of [8]):

$$\beta H^{an}(R) = \beta H^{an}(\beta, \mathbf{s}, \mathbf{t}) := -\frac{1}{n} \ln \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{s}, \mathbf{t}, \xi^n)}. \quad (168)$$

<sup>47</sup>Also, recall that the Teacher  $T$  is fixed and is not learned, so we do not integrate over  $d\mu(\mathbf{t})$ . In fact, for the (vector) Perceptron model, the Teacher  $T$  weights are simply subsumed into the overlap  $R$ , and even in the more general cases, such as non-Linear/Boolean Perceptron, in the full Replica calculations, etc. See the original literature for more details. [18, 8, 102] as well as [93].

where we have denoted the Hamiltonian as  $H^{an}(\beta, \mathbf{s}, \mathbf{t})$  to indicate the explicit dependence on  $\beta$ , and we have added  $\beta$  to the R.H.S. to because the L.H.S. is unitless. Using this definition, we can express the Annealed Partition Function,  $Z_n^{an}$ , in the AA in terms of the Annealed Hamiltonian  $H^{an}(R)$  (as in Eqn. 46 in Section 4.2, and as in Eqn. (2.31) of [8]):

$$Z_n^{an} := n \langle Z \rangle_{\xi^n} = \int d\mu(\mathbf{s}) e^{-n\beta H^{an}(\beta, \mathbf{s}, \mathbf{t})}. \quad (169)$$

Following Section 4.2.5, we can write the *Average Model Training Error*  $\bar{\mathcal{E}}_{train}^{ST}$ , in the AA, in terms of Annealed Partition Function,  $Z_n^{an}$ :

$$\bar{\mathcal{E}}_{train}^{ST} := -\frac{1}{n} \frac{\partial}{\partial \beta} \ln Z_n^{an} \quad (170)$$

This now lets us write the Average Model Training Error  $\bar{\mathcal{E}}_{train}^{ST}$  in the AA in terms of the Annealed Hamiltonian  $H^{an}(R)$ :

$$\begin{aligned} \bar{\mathcal{E}}_{train}^{ST} &= \frac{1}{Z_n^{an}} \int d\mu(\mathbf{s}) \frac{\partial \beta H^{an}}{\partial \beta} e^{-n\beta H^{an}(\beta, \mathbf{s}, \mathbf{t})} \\ &= \frac{1}{Z_n^{an}} \int d\mu(\mathbf{s}) \langle E_{\ell}^n(\mathbf{s}, \mathbf{t}, \xi) \rangle_{\xi^n} e^{-n\beta H^{an}(\beta, \mathbf{s}, \mathbf{t})}, \end{aligned} \quad (171)$$

where  $E_{\ell}^n(\mathbf{s}, \mathbf{t}, \xi)_{\xi^n}^{\beta}$  is a Thermal Average but defined over the specific ST error in the AA for the chosen set of training data  $\xi^{train} = \xi^n$ , and is denoted by

$$\langle E_{\ell}^n(\mathbf{s}, \mathbf{t}, \xi) \rangle_{\xi^n}^{\beta} := \frac{\partial \beta H^{an}}{\partial \beta}. \quad (172)$$

This is analogous to defining the average error  $E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)$  as a Thermal Average, but as one over the data  $\xi^n$  instead of the weights. This can be seen by expanding Eqn. 43, setting  $\mathbf{w} = \mathbf{s}$ , fixing  $\mathbf{t}$  (implicitly), and taking the partial derivative:

$$\begin{aligned} \frac{\partial \beta H^{an}}{\partial \beta} &= \frac{\partial}{\partial \beta} \left( -\frac{1}{n} \ln \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{w}, \xi^n)} \right) \\ &= -\frac{1}{n} \frac{\partial}{\partial \beta} \ln \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{w}, \xi^n)} \\ &= -\frac{1}{n} \left( \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{w}, \xi^n)} \right)^{-1} \frac{\partial}{\partial \beta} \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{w}, \xi^n)} \\ &= -\frac{1}{n} \left( \int d\mu(\xi^n) e^{-\beta E_{\ell_2}^n(\mathbf{w}, \xi^n)} \right)^{-1} \int d\mu(\xi^n) (-E_{\mathcal{L}}^n(\mathbf{w}, \xi^n)) e^{-\beta E_{\ell_2}^n(\mathbf{w}, \xi^n)} \end{aligned} \quad (173)$$

We can also write the Model Generalization Accuracy  $\bar{\mathcal{E}}_{gen}^{ST}$  as Boltzmann-weighted average of  $\epsilon(R)$ , weighted by  $H^{an}(\beta, S; T)$  (as in (2.32) in [8]), as:

$$\bar{\mathcal{E}}_{gen}^{ST} = \frac{1}{Z_n^{an}} \int d\mu(\mathbf{s}) \epsilon(R) e^{-n\beta H^{an}(\beta, \mathbf{s}, \mathbf{t})}, \quad (174)$$

where  $\epsilon(R) = \epsilon(\mathbf{s})$  is the average ST error, for a fixed Teacher T, averaged over *all* possible data inputs, i.e., not just over the specific training data. (Note that we have dropped the subscript *train* on  $\xi$  since it is clear from the context.)

In the high-T (small  $\beta$ ) limit, the two model errors become formally equivalent (i.e.,  $\bar{\mathcal{E}}_{train}^{ST} = \bar{\mathcal{E}}_{gen}^{ST}$  as  $T \rightarrow \infty$ ). To show this, consider the Annealed Hamiltonian  $H^{an}(R)$ , for the Linear

Perceptron with the  $\ell_2$  loss. As shown in Eqn. (C6) of [8], this takes a simple analytic form—in the Large- $\mathcal{N}$  limit in  $n$ —in terms of the ST overlap  $R$ :

$$H^{an}(R) = \frac{1}{2} \ln [1 + 2\beta(1 - R)]. \quad (175)$$

Eqn. 175 holds in the AA, but not in the High-T limit.

If we evaluate  $\frac{\partial H^{an}}{\partial \beta}$  in the High-T (small  $\beta$ ) limit, then we can use the approximation  $(\ln[1 + x] \simeq x + \dots)$  to obtain the High-T approximation:

$$\beta H^{an}(R) \simeq \beta H_{hT}^{an}(R) := \beta(1 - R), \quad \beta \text{ small.} \quad (176)$$

where we now see that  $H_{hT}^{an}(R)$  no longer explicitly depends on  $\beta$ . By Eqn. 49, this gives

$$\epsilon(R) = \langle \mathbf{E}_{\ell_2}(\mathbf{s}, \mathbf{t}, \boldsymbol{\xi}) \rangle_{\xi^n} \simeq 1 - R \text{ as } n \rightarrow \infty, \quad (177)$$

which we recognize as the same as the data-averaged ST error  $\epsilon(R)$  in Eqn. 97.

### A.2.2 Annealed Hamiltonian $H^{an}(\mathbf{R})$ for the Matrix-Generalized ST Error

In this section, we derive an expression for our matrix generalization of the Annealed Hamiltonian of the Linear Perceptron, in the AA and the high-T approximation, when student and teachers are modeled as  $N \times M$  matrices  $\mathbf{W}$ , i.e.,  $H^{an}(R) \rightarrow H^{an}(\mathbf{R})$ , which has the same form as Eqn. 168 for the vector case.

From this, we obtain an expression for the data-averaged ST error  $\epsilon(R)$ , again when the student and teachers are modeled as matrices. There is a subtle normalization issue here, about which we need to be careful. However, when we normalize appropriately, we will obtain an expression for “data-averaged ST error” (i.e., Annealed Error Potential)  $\epsilon(R)$  that is of the same form as we obtained in the vector case (as given in Eqn. 177 and Eqn. 97). The difference will be that in the vector case we take  $R = \frac{1}{N} \mathbf{s}^\top \mathbf{t}$ , while in the matrix case we take  $R = \frac{1}{N} \mathbf{S}^\top \mathbf{T}$ .

We will need to evaluate an average over the  $n$  random  $M$ -dimensional training data vectors  $\boldsymbol{\xi}^n$ , which are i.i.d Gaussian with 0 mean and  $\sigma^2$  variance:

$$\|\boldsymbol{\xi}^n\|^2 := \sum_{\mu=1}^n \boldsymbol{\xi}_\mu \boldsymbol{\xi}_\mu^\top = \sigma^2 \mathbf{I}_M, \quad (178)$$

where each  $\boldsymbol{\xi}_\mu$  is a vector of length  $M$ , and  $\mathbf{I}_M$  is an  $M \times M$  identity matrix. The expected value of the squared norm is:

$$\mathbb{E}[\|\boldsymbol{\xi}_\mu\|^2] = M\sigma^2. \quad (179)$$

If we let  $\sigma^2 \sim \frac{1}{M}$ , then  $\mathbb{E}[\|\boldsymbol{\xi}_\mu\|^2] = 1$ , i.e., the data vectors can be normalized to 1. Let the probability distribution over the  $N$  data vectors be

$$\begin{aligned} P(\boldsymbol{\xi}^n) &= \prod_{\mu=1}^n \left( \frac{1}{\sqrt{(2\pi\sigma^2)^M}} \right) e^{-\frac{\|\boldsymbol{\xi}_\mu\|^2}{2\sigma^2}} \\ &= \left( \frac{1}{\sqrt{(2\pi\sigma^2)^M}} \right)^n \exp \left[ -\frac{M}{2} \sum_{\mu=1}^n \|\boldsymbol{\xi}_\mu\|^2 \right] \\ &= \mathcal{N} \exp \left[ -\frac{M}{2} \sum_{\mu=1}^n \|\boldsymbol{\xi}_\mu\|^2 \right], \end{aligned} \quad (180)$$

where  $M = N_f$  is the number of features in the data, where the normalization  $\mathcal{N}$  is

$$\mathcal{N} := \left( \frac{1}{\sqrt{(2\pi\sigma^2)^M}} \right)^n = \left( \frac{M}{2\pi} \right)^{nM/2}. \quad (181)$$

3277 **The Total Data Sample Error ( $E_{\ell_2}^n(\mathbf{S}, \mathbf{T})$ ) and the Matrix Normalization** First, let us  
 3278 express the matrix-generalized Total Data Sample Error,  $E_{\ell_2}^n(\mathbf{S}, \mathbf{T})$ , for a single layer, in operator  
 3279 form (for each of the  $n$  training examples)

$$\frac{1}{n}E_{\ell_2}^n(\mathbf{S}, \mathbf{T}) := N \text{Tr} \left[ \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right] = NM - N \text{Tr}[\mathbf{R}] \quad (182)$$

3280 where  $\mathbf{I}_M$  is a diagonal matrix of dimension  $M$ . Note that the matrices are by default data-  
 3281 averaged empirical quantities, so we can drop the  $1/n$  on the RHS.

3282 Also, notice that  $E_{\ell_2}^n(\mathbf{S}, \mathbf{T})$  scales as  $N \times M$ , the total number of parameters in the system.  
 3283 Also, importantly, when all the overlaps are perfect, then the error is zero, i.e. if  $\text{Tr}[\mathbf{R}] = M$   
 3284 then  $E_{\ell_2}^n(\mathbf{S}, \mathbf{T}) = 0$ .

3285 We can define the data-dependent form (i.e., in the basis of the data  $\xi$ ) as

$$\begin{aligned} E_{\ell_2}^n(\mathbf{S}, \mathbf{T}, \xi^n) &:= N \sum_{\mu=1}^n (\xi^\mu)^\top \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) \xi^\mu \\ &= N \sum_{\mu=1}^n \sum_{i,j=1}^M \xi_i^\mu \left( \delta_{ij} - \frac{1}{N} [\mathbf{S}^\top \mathbf{T}]_{ij} \right) \xi_j^\mu. \end{aligned} \quad (183)$$

3286 **The Annealed Hamiltonian (per-parameter,  $h^{an}(\mathbf{R})$ )** The definition of the Annealed  
 3287 Hamiltonian,  $H^{an}(\mathbf{R})$ , for the idealized case must be extended to account for the  $N \times M$  pa-  
 3288 rameters per training example. We then have that the total energy is then the sum of the entries  
 3289 of  $M$  (feature) vectors, as expected by Size-Extensivity in  $N$  and Size-Consistency in  $M$ :

$$\text{Tr}[H^{an}(\mathbf{R})] = M (N \text{Tr}[h^{an}(\mathbf{R})]) \quad (184)$$

3290 where the Annealed Hamiltonian per-parameter,  $h^{an}(\mathbf{R})$ , is obtained from Eqn. 168 as

$$\begin{aligned} \beta h^{an}(\mathbf{R}) &:= -\frac{1}{n} \ln \int \mathcal{D}\xi^n e^{-\beta E_{\ell_2}^n(\mathbf{S}, \mathbf{T})} P(\xi^n) \\ &= -\frac{1}{n} \ln \mathbb{I}_H, \end{aligned} \quad (185)$$

3291 where

$$\mathbb{I}_H := \int \mathcal{D}\xi^n e^{-\beta E_{\ell_2}^n(\mathbf{S}, \mathbf{T})} P(\xi^n). \quad (186)$$

3292 That is,  $h^{an}(\mathbf{R})$  represents the Energy or Error that each of the  $N \times M$  parameters contributes  
 3293 (averaged over the  $N$  training examples  $\xi^n$ ).

3294 The goal will be to derive the high-Temperature Annealed Hamiltonian,  $H_{hT}^{an}(\mathbf{R})$ , which is  
 3295 now defined such that:

$$\text{Tr}[H_{hT}^{an}(\mathbf{R})] := MN (\text{Tr}[h_{hT}^{an}(\mathbf{R})]) \quad (187)$$

3296 If examining the the trace of  $h_{hT}^{an}(\mathbf{R})$ , then we can infer the functional form necessary to  
 3297 define the matrix-generalized Annealed Error Potential for each parameter:

$$\epsilon(\mathbf{R}) := \text{Tr}[h_{hT}^{an}(\mathbf{R})], \quad (188)$$

3298 which would be like a mean-field potential, but we need something different for the matrix case.



3299 To evaluate the integral, notice that  $\mathbb{I}_H$  is really just an average over i.i.d. data, and so it is  
 3300 just a product over  $n$  independent terms (1 for each training example).

$$\mathbb{I}_H := \int \mathcal{D}\xi^n e^{-\beta E_{\ell_2}^n(\mathbf{S}, \mathbf{T})} P(\xi^n) \rightarrow \left[ \int \mathcal{D}\xi [\dots] \right]^n, \quad (189)$$

3301 as in Eqn. 193 below. Moreover, when taking  $\ln \mathbb{I}_H$ , the  $N$  term pulls down and become a prefactor

$$-\ln \mathbb{I}_H = -\ln \left[ \int \mathcal{D}\xi [\dots] \right]^n = -n \ln \left[ \int \mathcal{D}\xi [\dots] \right]. \quad (190)$$

3302 Thus, as with the vector case,  $H^{an}(\mathbf{R})$  is like a mean-field average over the data  $\xi$ , independent  
 3303 of the sample size  $N$ . Also, since the final result must scale as  $N \times M$ , the integral should scale  
 3304 as  $M$ , i.e.,  $[\int \mathcal{D}\xi [\dots]] \sim M$ .

3305 If we substitute  $E_{\ell_2}^n(\mathbf{S}, \mathbf{T}, \xi^n)$ , Eqn. 183, into the integral  $\mathbb{I}_H$ , Eqn. 186, then we obtain

$$\mathbb{I}_H = \int \mathcal{D}\xi^n \exp \left( -\beta \sum_{\mu=1}^n N(\xi^\mu)^\top \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) \xi^\mu \right) P(\xi^n) \quad (191)$$

$$\begin{aligned} &= \int \mathcal{D}\xi^n \exp \left( -\beta \sum_{\mu=1}^n N(\xi^\mu)^\top \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) \xi^\mu \right) \mathcal{N} \exp \left( -\sum_{\mu=1}^N \frac{\|\xi^\mu\|^2}{2\sigma^2} \right) \\ &= \mathcal{N} \int \mathcal{D}\xi^n \exp \left( -\beta \sum_{\mu=1}^n N(\xi^\mu)^\top \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) (\xi^\mu) - \sum_{\mu=1}^n \frac{\|\xi^\mu\|^2}{2\sigma^2} \right) \\ &= \mathcal{N} \int \mathcal{D}\xi^n \exp \left( -\frac{1}{2\sigma^2} \sum_{\mu=1}^n 2\beta\sigma^2 N(\xi^\mu)^\top \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) (\xi^\mu) + \|\xi^\mu\|^2 \right) \\ &= \mathcal{N} \int \mathcal{D}\xi^n \exp \left( -\frac{1}{2\sigma^2} \sum_{\mu=1}^n (\xi^\mu)^\top [2\beta\sigma^2 N(\mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T}) + \mathbf{I}_M] (\xi^\mu) \right). \end{aligned} \quad (192)$$

3306 By combining the exponents, we obtain

$$\begin{aligned} \mathbb{I}_H &= \mathcal{N} \int \mathcal{D}\xi^n \exp \left[ -\frac{1}{2\sigma^2} \sum_{\mu=1}^N (\xi^\mu)^\top (\mathbf{M}) \xi^\mu \right] \\ &= \mathcal{N} \int \mathcal{D}\xi \exp \left[ -\frac{1}{2\sigma^2} (\xi)^\top (\mathbf{M}) \xi \right]^n, \end{aligned} \quad (193)$$

3307 where  $\mathbf{M} = 2\beta\sigma^2 N(\mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T}) + \mathbf{I}_M$  is an  $M \times M$  matrix. We now use the familiar property of  
 3308 multi-variant Gaussian integrals,

$$\int d\mathbf{x} e^{-\frac{1}{2\sigma^2} (\mathbf{x})^\top \mathbf{M} (\mathbf{x})} = (2\pi\sigma^2)^{M/2} \frac{1}{\sqrt{\det(\mathbf{M})}} \quad (194)$$

3309 where  $\mathbf{x}$  is an  $m$ -dim vector (with zero mean), and  $\mathbf{M}$  is a square positive-definite matrix, and  
 3310  $\det(\mathbf{M})$  is the determinant of  $\mathbf{M}$ . Using Eqn. 194, we can rewrite  $\mathbb{I}_H$  in Eqn. 193 as

$$\mathbb{I}_H = \mathcal{N} \left[ \frac{(2\pi\sigma^2)^{M/2}}{\sqrt{\det(\mathbf{M})}} \right]^n \quad (195)$$

$$\begin{aligned} &= \mathcal{N} (2\pi\sigma^2)^{NM/2} \left[ \sqrt{\det(2\beta\sigma^2 N(\mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T}) + \mathbf{I}_M)} \right]^{-n} \\ &= \left( \frac{1}{2\pi\sigma^2} \right)^{NM/2} (2\pi\sigma^2)^{M/2} \left[ \sqrt{\det(\mathbf{I}_M + 2\beta\sigma^2 N(\mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T}))} \right]^{-n}, \end{aligned} \quad (196)$$

where Eqn. 196 follows by inserting  $\mathcal{N}$  from Eqn. 181. We can now identify  $\sigma^2 = \frac{1}{M}$  to obtain

$$\begin{aligned}\mathbb{I}_H &= \left[ \sqrt{\det \left( \mathbf{I}_M + 2\beta\sigma^2 N \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) \right)} \right]^{-n} \\ &= \left[ \sqrt{\det \left( \mathbf{I}_M + \frac{2\beta}{M} N \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) \right)} \right]^{-n} \\ &= \left[ \det \left( \mathbf{I}_M + \frac{2\beta}{M} N \left( \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right) \right) \right]^{-n/2}.\end{aligned}\quad (197)$$

**The High-Temperature Limit.** In the high-T approximation,  $\beta$  becomes small, giving the expression  $\det(\mathbf{I}_M + \epsilon \mathbf{\Omega}) \approx 1 + \epsilon \text{Tr}[\mathbf{\Omega}]$ , which holds for an arbitrary matrix  $\mathbf{\Omega}$  for small  $\epsilon$ . Using this, we can evaluate the determinant in Eqn. 197 in the large- $N$  approximation, which gives

$$\mathbb{I}_H \approx \left[ 1 + \frac{2\beta}{M} N \left( \text{Tr} \left[ \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right] \right) \right]^{-n/2}. \quad (198)$$

Inserting this into Eqn. 185, we obtain

$$\begin{aligned}\beta h^{an}(\mathbf{R}) &= -\frac{1}{n} \ln \left[ 1 + \frac{2\beta}{M} N \left( \text{Tr} \left[ \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right] \right) \right]^{-n/2} \\ &= \frac{1}{2} \ln \left[ 1 + \frac{2\beta}{M} N \left( \text{Tr} \left[ \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right] \right) \right]\end{aligned}\quad (199)$$

This form of the Hamiltonian,  $H^{an}(\mathbf{R})$ , however, is not symmetric, and we will eventually want a symmetric operator or matrix. Fortunately, the high-T form,  $H_{hT}^{an}(\mathbf{R})$ , can be made symmetric, as shown below. But first, let show that this result is consistent with the our previous Percpetron result.

**Matrix-Generalized ST Error  $H_{hT}^{an}(\mathbf{R})$  for  $N = 1$ .** To start, observe that when  $N = 1$ , Eqn. 200 becomes

$$\begin{aligned}\beta H^{an}(\mathbf{R})|_{N=1} &= \beta h^{an}(\mathbf{R})|_{N=1} \\ &= -\frac{1}{n} \ln \left[ 1 + 2\beta \frac{1}{M} \text{Tr} \left[ (M - \mathbf{s}^\top \mathbf{t}) \right] \right]^{-n/2}\end{aligned}\quad (200)$$

$$\begin{aligned}&= \frac{1}{2} \ln \left[ 1 + 2\beta \frac{1}{M} \text{Tr} \left[ M - \mathbf{s}^\top \mathbf{t} \right] \right] \\ &= \frac{1}{2} \ln \left[ 1 + 2\beta(1 - R) \right],\end{aligned}\quad (201)$$

where we recall that  $\mathbf{s}$  and  $\mathbf{t}$  are implicitly normalized to  $1/m$ , where here  $m = M$ . This result shows that Eqn. 200 reduces to Eqn. 175, as desired.

This ensures the Hamiltonian scales as  $M$  so the Free Energy scales as  $N \times M$ , the number of free paramaters in the system. Notice that for the final Layer Quality-Squared Hamiltonian  $\mathbf{H}_{\tilde{Q}^2}$ , this will change.

$$\mathbb{I}_H \approx \left[ 1 + \frac{2\beta}{M} N \text{Tr} \left[ \mathbf{I}_M - \frac{1}{N} \mathbf{S}^\top \mathbf{T} \right] \right]^{-n/2}, \quad (202)$$

for any  $M > 1$ . Given this, it follows from Eqn. 200 and Eqn. 185 that we can define

$$\beta H^{an}(\mathbf{R})|_{N=1} := \frac{M}{2} \ln \det \left[ 1 + \frac{2\beta}{M} (\mathbf{I}_M - \mathbf{R}) \right], \quad (203)$$

and reduces to the same functional form as Eqn. 175, as desired (recalling that  $\mathbf{s}$  and  $\mathbf{t}$  are implicitly normalized by  $M = m$ ).

To obtain the high-Temperature form, we use

$$\ln \det[\mathbf{I}_M + \epsilon \mathbb{M}] \approx \text{Tr}(\epsilon \mathbb{M}) \quad (\epsilon \ll 1), \quad (204)$$

with  $\epsilon = \frac{2\beta}{M}$  and  $\mathbb{M} = \mathbf{I}_M - \mathbf{R}$ . We now obtain the following result for the matrix-generalized high-T of  $H_{hT}^{an}(\mathbf{R})$  using

$$\text{Tr}[H_{hT}^{an}(\mathbf{R})]|_{N=1} = \text{Tr}[\mathbf{I}_M - \mathbf{R}] = M - \text{Tr}[\mathbf{R}] \quad (205)$$

The final expression for  $H_{hT}^{an}(\mathbf{R})$  is

$$H_{hT}^{an}(\mathbf{R}) = N(\mathbf{I}_M - \mathbf{R}) \quad (206)$$

### A.3 Expressing the Layer Quality

In this section, we obtain an approximation expression for the Layer Quality-Squared from the IZ Free Energy for the Generalization Error, given in Eqn. 113 in Section 5.2.1.

For the required Free Energy  $\beta \mathbf{F}^{IZ}$ , we will use the matrix-generalized Hamiltonian from Eqn. 206 for the Layer Quality,  $H_{hT}^{an}(\mathbf{R}) = N(\mathbf{I}_M - \mathbf{R})$ . giving a Boltzmann distribution and the corresponding Thermal Average. Expanding this out, we have

$$-\beta \mathbf{F}^{IZ} = -\ln \int d\mu(\mathbf{S}) \exp[-n\beta \text{Tr}[H_{hT}^{an}(\mathbf{R})]] \quad (207)$$

$$(208)$$

We could also express  $\beta \mathbf{F}^{IZ}$  In terms of the matrix-generalized Annealed Error Potential  $\epsilon(\mathbf{R})$  (Eqn. 188), giving

$$-\beta \mathbf{F}^{IZ} = -\ln \int d\mu(\mathbf{S}) \exp[-n\beta N \epsilon(\mathbf{R})] \quad (209)$$

In analogy with Eqn. 49, as  $H_{hT}^{an}(\mathbf{R}) = M - \mathbf{R}$ , write

$$-\beta \mathbf{F}^{IZ} = -\ln \int d\mu(\mathbf{S}) \exp[-n\beta N \text{Tr}[M - \mathbf{R}]] \quad (210)$$

Using the approximation  $\text{Tr}[\mathbf{R}] \approx \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]}$ , we have

$$-\beta \mathbf{F}^{IZ} \approx -\ln \int d\mu(\mathbf{S}) \exp[-n\beta N (M - \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]})] \quad (211)$$

$$= -\ln \int d\mu(\mathbf{S}) \exp[-n\beta N M] \exp[n\beta N \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]}], \quad (212)$$

$$= -\ln e^{-n\beta N M} \int d\mu(\mathbf{S}) \exp[n\beta N \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]}], \quad (213)$$

$$= -\ln e^{-n\beta N M} - \ln \int d\mu(\mathbf{S}) \exp[n\beta N \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]}], \quad (214)$$

$$= n\beta N M - \ln \int d\mu(\mathbf{S}) \exp[n\beta N \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]}], \quad (215)$$

Notice that, as expected, the Free Energy scales  $\beta \mathbf{F}^{IZ}$  as  $n \times N \times M$ , the total number of degrees of freedom of the theory. Since Eqn. 207 equals Eqn. 212, we can write the Free Energy

in terms of  $\text{Tr}[\mathbf{R}^\top \mathbf{R}]$ . From Eqn. 215, we can identify a generating function ( $\Gamma_{\bar{Q}}$ ) for the layer accuracy, or Quality. For example, to compute the average Quality  $\bar{Q}$ , we would use

$$\beta \Gamma_{\bar{Q}}^{IZ} := \ln \int d\mu(\mathbf{S}) \exp \left[ n\beta N \sqrt{\text{Tr}[\mathbf{R}^\top \mathbf{R}]} \right], \quad (216)$$

and to compute the average Quality (squared)  $\bar{Q}^2$ , we would use

$$\beta \Gamma_{\bar{Q}^2}^{IZ} := \ln \int d\mu(\mathbf{S}) \exp \left[ n\beta N \text{Tr}[\mathbf{R}^\top \mathbf{R}] \right]. \quad (217)$$

We have recovered Eqn. 113. We can now also define the Layer Quality-Squared Hamiltonian as

$$\mathbf{H}_{\bar{Q}^2} := \mathbf{R}^\top \mathbf{R} \quad (218)$$

which is a symmetric operator, as desired. Consequently, we may also write

$$\beta \Gamma_{\bar{Q}^2}^{IZ} := \ln \int d\mu(\mathbf{S}) \exp \left[ n\beta N \text{Tr}[\mathbf{H}_{\bar{Q}^2}] \right]. \quad (219)$$

## A.4 Derivation of the ERG Condition

### A.4.1 Setting up the Saddle Point Approximation (SPA)

As in Eqn. 118, we can write Eqn. 11 in terms of the  $\mathbf{A}_N = \mathbf{S}\mathbf{S}^\top$  form of the Outer Student Correlation matrix, giving

$$\beta \Gamma_{\bar{Q}^2}^{IZ} = \ln \int_{\mathbf{S}} d\mu(\mathbf{S}) \exp \left( n\beta N \text{Tr} \left[ \frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T} \right] \right) \quad (220)$$

where  $d\mu(\mathbf{S})$  is the measure over all  $N \times M$  real-valued random matrices, although we really want to limit this to all  $N \times M$  real matrices that resemble the Teacher  $\mathbf{T}$ , which we clarify below.

To transform  $\beta \Gamma_{\bar{Q}^2}^{IZ}$  into a form we can evaluate using Tanaka's result [84], we need to change the measure from an integral over all random  $N \times M$  student weight matrices  $d\mu(\mathbf{S})$  to an integral over all  $N \times N$  student correlation matrices  $d\mu(\mathbf{A}_M)$ , i.e.,  $d\mu(\mathbf{S}) \rightarrow d\mu(\mathbf{A}_M)$ . To accomplish this, we can insert an integral over the Dirac Delta function

$$\mathbf{I} := \int d\mu(\mathbf{A}_M) \delta(N\mathbf{A}_M - \mathbf{S}^\top \mathbf{S}). \quad (221)$$

(This is simply a resolution of the Identity.) This gives

$$\beta \Gamma_{\bar{Q}^2}^{IZ} = \ln \int_{\mathbf{S}} d\mu(\mathbf{S}) \int_{\mathbf{A}} d\mu(\mathbf{A}_M) \delta(N\mathbf{A}_M - \mathbf{S}^\top \mathbf{S}) e^{n\beta N \text{Tr} \left[ \frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T} \right]}, \quad (222)$$

where  $d\mu(\mathbf{A}) = \mathbf{Pr}[\mathbf{A}] d\mathbf{A}$  and  $\mathbf{Pr}[\mathbf{A}]$  is the (still unspecified) probability density over the new random matrix  $\mathbf{A}$ . Let us express Eqn. 222 at Large- $\mathcal{N}$  limit in  $N$  as

$$\lim_{N \gg 1} \beta \Gamma_{\bar{Q}^2}^{IZ} = \lim_{N \gg 1} \ln \int d\mu(\mathbf{A}) \int d\mu(\mathbf{S}) \delta(N\mathbf{A}_M - \mathbf{S}^\top \mathbf{S}) e^{n\beta N \text{Tr} \left[ \frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T} \right]}. \quad (223)$$

Now we assume we can first evaluate the term

$$\lim_{N \gg 1} \int d\mu(\mathbf{S}) \delta(N\mathbf{A}_M - \mathbf{S}^\top \mathbf{S}) \quad (224)$$

at Large- $\mathcal{N}$  in  $N$  using a Saddle Point Approximation (SPA). Using the relation,

$$\delta(N\mathbf{A}_M - \mathbf{S}^\top \mathbf{S}) = \mathcal{N}_M \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{iN \text{Tr}[\hat{\mathbf{A}} \mathbf{A}_M]} e^{-i \text{Tr}[\hat{\mathbf{A}} \mathbf{S}^\top \mathbf{S}]}, \quad (225)$$

where  $\hat{\mathbf{A}}$  is an  $M \times M$  auxiliary matrix, and the domain of integration  $d\mu(\hat{\mathbf{A}})$  is all  $M \times M$  real-valued matrices, and where the normalization  $\mathcal{N}_1$  is

$$\mathcal{N}_1 := \frac{1}{(2\pi)^{M(M+1)/4}}, \quad (226)$$

because  $\mathbf{A}$  is a symmetric matrix with  $M(M+1)/2$  constraints.

This is simply the matrix generalization of  $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\hat{x}x} d\hat{x}$ , so we can express the delta function as an exponential, giving

$$\beta\Gamma_{\mathcal{Q}^2}^{IZ} = \mathcal{N}_1 \ln \int_{\mathbf{S}} d\mu(\mathbf{S}) \int_{\mathbf{A}} d\mu(\mathbf{A}_M) \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{iN\text{Tr}[\hat{\mathbf{A}}\mathbf{A}_M]} e^{-i\text{Tr}[\hat{\mathbf{A}}\mathbf{S}^\top\mathbf{S}]} e^{n\beta N\text{Tr}[\frac{1}{N}\mathbf{T}^\top\mathbf{A}_N\mathbf{T}]}. \quad (227)$$

Rearranging terms, we obtain

$$\beta\Gamma_{\mathcal{Q}^2}^{IZ} = \ln \int_{\mathbf{A}} d\mu(\mathbf{A}_M) e^{n\beta N\text{Tr}[\frac{1}{N}\mathbf{T}^\top\mathbf{A}_N\mathbf{T}]} \times \Gamma_1, \quad (228)$$

where we define  $\Gamma_1$  as

$$\Gamma_1 := \Gamma_1(\mathbf{A}_M) = \mathcal{N}_1 \int_{\mathbf{S}} d\mu(\mathbf{S}) \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{iN\text{Tr}[\hat{\mathbf{A}}\mathbf{A}_M]} e^{-i\text{Tr}[\hat{\mathbf{A}}\mathbf{S}^\top\mathbf{S}]}. \quad (229)$$

We can simplify the complex integral in  $\Gamma_1$  with the Wick Rotation  $i\hat{\mathbf{A}} \rightarrow \hat{\mathbf{A}}$ . The Wick rotation ensures that the Gaussian integral converges (although this has not been rigorously checked). We may expect  $d\mu(\hat{\mathbf{A}})$  to be invariant to rotations in the complex plane, so the Wick rotation does not introduce any complex prefactors. This gives

$$\Gamma_1 = \mathcal{N}_1 \int_{\mathbf{S}} d\mu(\mathbf{S}) \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{N\text{Tr}[\hat{\mathbf{A}}\mathbf{A}_M]} e^{-\text{Tr}[\hat{\mathbf{A}}\mathbf{S}^\top\mathbf{S}]} \quad (230)$$

$$= \mathcal{N}_1 \int_{\mathbf{S}} d\mu(\mathbf{S}) \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{N\text{Tr}[\hat{\mathbf{A}}\mathbf{A}_M]} e^{-\text{Tr}[\mathbf{S}\hat{\mathbf{A}}\mathbf{S}^\top]}, \quad (231)$$

where the second line follows since the trace is invariant under cyclic permutations (i.e.,  $\text{Tr}[ABC] = \text{Tr}[BCA] = \text{Tr}[CAB]$ ). Swapping the order of the integrals yields

$$\Gamma_1 = \Gamma_1(\hat{\mathbf{A}}) = \mathcal{N}_1 \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{N\text{Tr}[\hat{\mathbf{A}}\mathbf{A}_M]} \times \Gamma_2, \quad (232)$$

where we define  $\Gamma_2$  as

$$\Gamma_2 := \Gamma_2(\hat{\mathbf{A}}) = \int_{\mathbf{S}} d\mu(\mathbf{S}) e^{-\text{Tr}[\mathbf{S}\hat{\mathbf{A}}\mathbf{S}^\top]}.$$

To evaluate  $\Gamma_2$ , we will make several mathematically convenient approximations. (These will yield an approximate expression which can be verified empirically.) We first assume for the purpose of changing measure that the (data) columns of  $\mathbf{S}$  are statistically independent, so that the measure  $d\mu(\mathbf{S})$  factors into  $N$  Gaussian distributions

$$d\mu(\mathbf{S}) = \prod_{\mu=1}^N d\mu(\mathbf{s}_\mu) = \prod_{\mu=1}^N d\mathbf{s}_\mu, \quad (233)$$

where  $\mathbf{s}_\mu$  is an  $M$ -dimensional vector. The singular values of  $\mathbf{S}$  are invariant to random permutations of the columns or rows, so the resulting ESD does not change. This is very different from permuting  $\mathbf{S}$  element-wise, which will make the resulting ESD Marchenko Pastur (MP).

Using Eqn. 233,  $\Gamma_2$  reduces to a simple Gaussian integral, which can be evaluated as a product of  $N$  Gaussian integrals (over the  $M \times M$  matrix  $\hat{\mathbf{A}}$ )

$$\Gamma_2 = \left[ \int_{\mathbf{s}} d\mathbf{s} e^{-\frac{1}{\sigma^2} \mathbf{s} \hat{\mathbf{A}} \mathbf{s}^\top} \right]^N \quad (234)$$

$$= \left[ \mathcal{N}_2 \det(\hat{\mathbf{A}})^{-1/2} \right]^N, \quad (235)$$

where the normalization term  $\mathcal{N}_2$

$$\mathcal{N}_2 := (\pi \sigma^2)^{M/2}, \quad (236)$$

where  $\sigma^2 = \mathbf{s}^\top \mathbf{s} = 1/M$

For any square, non-singular matrix  $\hat{\mathbf{A}}$ ,  $\text{Tr}[\ln \hat{\mathbf{A}}] = \ln \det(\hat{\mathbf{A}})$ , so it follows from Eqn. 234 that

$$\begin{aligned} \ln \Gamma_2 &= N \ln \mathcal{N}_2 \left[ (\det(\hat{\mathbf{A}}))^{-1/2} \right] \\ &= N \ln \mathcal{N}_2 - \frac{N}{2} \text{Tr}[\ln \hat{\mathbf{A}}], \end{aligned} \quad (237)$$

so that

$$\Gamma_2 = (\mathcal{N}_2)^N e^{-\frac{N}{2} \text{Tr}[\ln \hat{\mathbf{A}}]} \quad (238)$$

Substituting Eqn. 238 into Eqn. 232, we can write  $\Gamma_1$  as

$$\Gamma_1(\hat{\mathbf{A}}) = C_{\Gamma_1} \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{N \text{Tr}[\hat{\mathbf{A}} \mathbf{A}_M]} e^{-\frac{N}{2} \text{Tr}[\ln \hat{\mathbf{A}}]}, \quad (239)$$

where

$$C_{\Gamma_1} := \mathcal{N}_1 e^{\mathcal{N}_2}. \quad (240)$$

We can now evaluate the integral in Eqn. 232 over the Lagrange multiplier  $\hat{\mathbf{A}}$  (i.e.,  $\int_{\hat{\mathbf{A}}}$ ). If we call this  $\Gamma_1(\hat{\mathbf{A}})$ , then (following Tanaka [84]) we can define the *Rate Function*  $I(\hat{\mathbf{A}}, \mathbf{A}_M)$  such that

$$\Gamma_1(\hat{\mathbf{A}}) = \int_{\hat{\mathbf{A}}} d\mu(\hat{\mathbf{A}}) e^{-NI(\hat{\mathbf{A}}, \mathbf{A}_M)}, \quad (241)$$

where

$$I(\hat{\mathbf{A}}, \mathbf{A}_M) = -\text{Tr}[\hat{\mathbf{A}} \mathbf{A}_M] + \frac{1}{2} \text{Tr}[\ln \hat{\mathbf{A}}]. \quad (242)$$

We can formally evaluate the integral in Eqn. 241 in the large- $N$  limit using a Saddle Point Approximation (SPA) (see Section 4.2, Eqn. 68), as

$$\Gamma_1(\hat{\mathbf{A}}) \rightarrow \sqrt{\frac{(2\pi)^{N/2}}{N \|I\|}} e^{-NI^*(\hat{\mathbf{A}}, \mathbf{A}_M)}, \quad (243)$$

where  $I^*(\hat{\mathbf{A}}, \mathbf{A}_M)$  is the maximum value over all  $\hat{\mathbf{A}}$  for fixed  $\mathbf{A}_M$ , obtained using

$$I^*(\hat{\mathbf{A}}, \mathbf{A}_M) := \lim_{N \gg 1} I(\hat{\mathbf{A}}, \mathbf{A}_M) = \sup_{\hat{\mathbf{A}}} \left[ -\text{Tr}[\hat{\mathbf{A}} \mathbf{A}_M] + \frac{1}{2} \text{Tr}[\ln \hat{\mathbf{A}}] \right], \quad (244)$$



where at the SPA we have stationarity,

$$\frac{\partial}{\partial \hat{\mathbf{A}}} I(\hat{\mathbf{A}}, \mathbf{A}_M) = -\mathbf{A}_M + \frac{1}{2\hat{\mathbf{A}}} = 0 \quad (245)$$

and the Hessian of  $I$  becomes

$$\frac{\partial^2}{\partial \hat{\mathbf{A}}^2} I(\hat{\mathbf{A}}, \mathbf{A}_M) = -\frac{1}{2} \left( \frac{1}{2} \hat{\mathbf{A}}^{-1} \right) \otimes \left( \frac{1}{2} \hat{\mathbf{A}}^{-1} \right) = -\frac{1}{8} \mathbf{A}_M \otimes \mathbf{A}_M \quad (246)$$

where  $\otimes$  is the Kronecker product. Using Eqn. 245, we have that  $1/8 \mathbf{A}_M \otimes \mathbf{A}_M$  is the saddle point Hessian of  $I$  w.r.t.  $\mathbf{A}_M$ . Solving the SPA equation, we find that the prefactor (i.e. Hessian) is given as  $\det(-\frac{1}{8} \mathbf{A}_M \otimes \mathbf{A}_M) = (-\frac{1}{8})^{M^2} (\det(\mathbf{A}_M))^M$ .

Substituting for  $\hat{\mathbf{A}}$  into Rate Function (Eqn. 242),  $I$  becomes

$$\begin{aligned} I^*(\hat{\mathbf{A}}, \mathbf{A}_M) &= -\text{Tr}[\mathbf{I}_M] + \frac{1}{2} \text{Tr}[\ln \mathbf{A}_M] \\ &= -M + \frac{1}{2} \text{Tr}[\ln \mathbf{A}_M]. \end{aligned} \quad (247)$$

In order for this result to be physically meaningful, we need that if  $I^*(\hat{\mathbf{A}}, \mathbf{A}_M)$  grows, then it must grow slower than  $N$ , and, more importantly, that  $\det(\mathbf{A})$  be non-zero. Importantly, when  $\det(\mathbf{A}) = 1$  exactly, however, then  $\Gamma_1$  becomes a constant, and this simplifies things considerably!

#### A.4.2 Casting the Generating Function ( $\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}$ ) as an HCIZ Integral

In this section, we express the Generating Function  $\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}$ , given in Eqn. 118 (equivalently, in Eqn. 113,) as an HCIZ Integral, as given in Eqn. 122.

Inserting  $I^*(\hat{\mathbf{A}}, \mathbf{A})$  from Eqn. 247 into  $\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}$ , we obtain

$$\begin{aligned} \beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ} &= \ln \left[ C_{\Gamma_1} e^{-NM} \int d\mu(\mathbf{A}) e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\mathbf{A}_M))} \right] \\ &= \ln C_{\Gamma_1} - NM + \ln \left[ \int d\mu(\mathbf{A}) e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\mathbf{A}_M))} \right]. \end{aligned} \quad (248)$$

So long as the second term  $\text{Tr}[\mathbf{I}_M]$  does not depend on  $N$ , it will vanish when we take the partial derivative of  $\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}$  to obtain the  $\tilde{\mathcal{E}}_{gen}^{NN}$ , in which case it is not important. We can then simply write the Generating Function  $\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ}$  as in Eqn. 119 as:

$$\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ} = \ln \left[ \int d\mu(\mathbf{A}_M) e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\mathbf{A}_M))} \right], \quad (249)$$

or, in Bra-Ket notation, as

$$\beta \Gamma_{\tilde{\mathcal{Q}}^2}^{IZ} = \ln \left\langle e^{n\beta N \text{Tr}[\frac{1}{N} \mathbf{T}^\top \mathbf{A}_N \mathbf{T}]} e^{\frac{N}{2} \ln(\det(\mathbf{A}_M))} \right\rangle_{\mathbf{A}_M}. \quad (250)$$

## A.5 MLP3 Model Details

The empirical MLP3 Model implements the assumptions described in Section 5 used the following procedures:

A three-layer Multi-Layer Perceptron was trained for classification on the MNIST dataset[117]. The first Fully Connected (FC) hidden layer has 300 units, the second FC hidden layer has 100

units, and the third FC layer has ten units for classification, matching the ten digit classes of MNIST. Input images are grayscale, and were rescaled to the  $[0, 1]$  range. Following the keras[130] defaults, the weights were initialized using the Glorot Normal[131] method, and the biases were initialized to 0. Each model was trained using Categorical Cross Entropy as the loss function. The loss function was *summed* over each mini-batch, which is the default behavior for Keras, rather than being *averaged*, which is the default for pytorch[132].

Optimization was carried out by either Stochastic Gradient Descent (SGD) without momentum, or the Adam algorithm [133]. The Learning Rate (LR) was set to 0.01 for SGD, and 0.001 for Adam. The LR was held constant, i.e., there was no decay schedule. Each algorithm proceeded epoch by epoch until the value of the loss function did not decrease by more than 0.0001 for three consecutive epochs. At each epoch, the `WeightWatcher` tool was used to compute metrics for each layer. Loss values reported are the average loss per labeled example, and not the summed loss over each minibatch. Training loss is averaged over all batches in the epoch, whereas test loss is evaluated once at the end of the epoch.

In some experiments, only one layer was trained, while the others were left frozen. In other experiments all layers were trained. Models were trained using a series of mini-batch sizes ranging from 1 to 32. For each separate training run, the models were re-initialized to the same starting random weights, all random seeds were reset, and deterministic computations were used to train the models.

Separate notebooks are provided for keras and pytorch implementations of the experiments.

## A.6 Tanaka’s Result

In this section, we will rederive the result by Tanaka [83, 84] that we use in our main derivation, and, importantly, explain how to address the missing Temperature term. For completeness, we restate it here using the notation of the main text:

$$\lim_{N \gg 1} \frac{1}{N} \ln \underbrace{\left( \exp \left( \frac{n\beta}{2} \text{Tr} [\mathbf{W}^\top \mathbf{A}_N \mathbf{W}] \right) \right)}_{\text{HCIZ Integral}} \Big|_{\mathbf{A}} = \frac{n\beta}{2} \sum_{i=1}^M \mathbb{G}_{\mathbf{A}}(\lambda_i) \quad (251)$$

where  $\mathbf{W}$  is the  $N \times M$  Teacher weight matrix,  $\mathbf{A} = \mathbf{A}_N$  is the  $N \times N$  Student (correlation) matrix, but  $\beta$  is now the inverse-Temperature (because we are working with real matrices),  $n$  is the size of the training set, and we have added the  $(\frac{1}{2})$  prefactor (which will be clear later).  $\mathbb{G}_{\mathbf{A}}(\lambda)$  is a complex analytic function of the eigenvalues  $\lambda$  of (the Teacher Correlation matrix)  $\mathbf{X}$ , whose functional form will depend on the structure of the limiting form of (the Student) ESD  $\rho_{\mathbf{A}}^\infty(\lambda)$ . We may also write it as  $\mathbb{G}_{\mathbf{A}}(\mathbf{X})$  below. We call it perhaps somewhat imprecisely a *Norm Generating Function* because the final results for the Layer Quality  $\bar{\mathcal{Q}}$  will take the form of a *Tail norm* in many cases.

To apply this result, we note that while the term  $\beta$  is just a constant in [84] (1 or 2, depending on whether the random matrix is real or complex), it is not actually inverse Temperature  $\beta = \frac{1}{T}$  in the original derivation. Still, we seek a final result that is linear in  $\beta = \frac{1}{T}$ , so that we can easily evaluate  $\bar{\mathcal{Q}}^2$  in the high-T limit, i.e.  $\bar{\mathcal{Q}}^2 = \frac{\partial}{\partial n} \frac{1}{\beta} \beta \mathbf{\Gamma}_{\bar{\mathcal{Q}}^2, N \gg 1}^{IZ} = \frac{\partial}{\partial \beta} \frac{1}{n} \beta \mathbf{\Gamma}_{\bar{\mathcal{Q}}^2, N \gg 1}^{IZ}$  (see 11). We can introduce the new term  $n\beta$  by simply changing the scale of  $\mathbf{A}_N$  since the final result is a sum of R-transforms, which by definition are linear, i.e.,  $\mathbb{G}_{\mathbf{A}}(n\beta\lambda) = n\beta\mathbb{G}_{\mathbf{A}}(\lambda)$ , however, it is instructive to rederive the final result, with  $n\beta$  explicitly included.

3464 **Notation.** We start by rewriting the Tanaka result, Eqn. (251), in our notation for the expected  
 3465 value  $\langle \dots \rangle_{\mathbf{A}}$  operator, as follows:

$$\frac{1}{2N} \beta \Gamma_{\bar{Q}^2, N \gg 1}^{IZ} = \frac{1}{N} \lim_{N \gg 1} \ln \underbrace{\int d\mu(\mathbf{A}) \left[ \exp \left( \frac{n\beta}{2} \text{Tr} [\mathbf{W}^\top \mathbf{A}_N \mathbf{W}] \right) \right]}_{\text{HCIZ Integral}} = n\beta \frac{1}{2} \sum_{i=1}^M \mathbb{G}_{\mathbf{A}}(\lambda_i). \quad (252)$$

3466 where we have added a  $\frac{1}{2}$  for technical convenience (to make the connection with the LDP, below).  
 3467 If we denote the internal HCIZ integral as

$$\mathbb{Z}^{IZ} := \int d\mu(\mathbf{A}) \left[ \exp \left( \frac{n\beta}{2} \text{Tr} [\mathbf{W}^\top \mathbf{A}_N \mathbf{W}] \right) \right], \quad (253)$$

3468 then it holds that

$$\beta \Gamma_{\bar{Q}^2}^{IZ} := \frac{1}{N} \ln \mathbb{Z}^{IZ}, \quad (254)$$

3469 from which it follows that

$$\beta \Gamma_{\bar{Q}^2, N \gg 1}^{IZ} := \lim_{N \gg 1} \frac{1}{N} \ln \mathbb{Z}^{IZ}. \quad (255)$$

3470 The SPA approximates the Partition Function  $\mathbb{Z}^{IZ}$ , which is now an HCIZ integral, by its  
 3471 peak value. For this,  $\mathbb{G}_{\mathbf{A}}(\lambda)$  itself must either not explicitly depend on  $N$  and/or at least not  
 3472 grow faster than  $N$ .

3473 The trick here is we can choose an R-transform of  $\mathbf{A}$  that is a simple analytic expression based  
 3474 on the observed empirical spectral density (ESD) of the  $\mathbf{X}$ . And this can readily be done for the  
 3475 ESDs for a wide range of layer weight matrices observed in modern DNNs because their ESDs are  
 3476 Heavy-Tailed Power Law [63]. We can then readily express the Quality  $\bar{Q}$  of the Teacher layer in  
 3477 a simple functional form, (i.e an approximate Shatten Norm).

3478 Importantly, the matrices  $\mathbf{X}$  and  $\mathbf{A}$  must be well approximated by low rank matrices since  
 3479 the derivation in Tanaka requires this. Fortunately, this appears to be generally true for the  
 3480 layers in very well trained DNNs, which is what allows us to apply this withing the ECS. In fact,  
 3481 technically we need to integrate over  $d\mu(\tilde{\mathbf{A}})$ ; this is straightforward as this simply changes the  
 3482 lower bound on the integral from  $0 \rightarrow \tilde{\lambda}_{min}$ , both above and in the subsequent derivation.

3483 Finally, we note that  $\mathbb{G}_{\mathbf{A}}(\mathbf{X})$  is kind of *Generalized Norm* because it can be evaluated as a  
 3484 sum over a function of the  $M$  eigenvalues  $\lambda_\mu$  of the Teacher correlation matrix  $\mathbf{X} = \frac{1}{N} \mathbf{W}^\top \mathbf{W}$ .  
 3485  $\mathbb{G}_{\mathbf{A}}(\mathbf{X})$  will turn out to be an expression similar to the Frobenius Norm or the Shatten Norm  
 3486 of  $\mathbf{X}$ , depending on the functional form we choose to represent the limiting form of the Student  
 3487 ESD,  $\rho_{\mathbf{A}}^\infty(\lambda)$  and the associated R-transform  $R(z)$ , and various approximations made thereafter,

### 3488 A.6.1 Setup and Outline

3489 To evaluate 252, we want to integrate over all Student Correlation matrices  $\mathbf{A}$  that “resemble”  
 3490 the Teacher Correlation matrix  $\mathbf{X}$ . To formalize this idea, we need to define the measure over “all  
 3491 desired”  $\mathbf{A}$ ,  $d\mu(\mathbf{A})$ , in terms of the actual  $M$  eigenvalues,  $\{\lambda_i\}_{i=1}^M$ , of the Teacher. And WLOG,  
 3492 the final result can be restricted to the  $\tilde{M}$  eigenvalues of the Effective Correlation Space (ECS).

3493 **Randomness assumption.** For real weights  $\mathbf{W}$ , we assume an *orthogonally invariant* ensemble,  
 3494  $d\mu(\mathbf{W}) = d\mu(\mathbf{U}\mathbf{W}\mathbf{U}^\top)$  for all  $\mathbf{U} \in O(M)$ , mirroring the isotropic Gaussian initialisation  
 3495 widely used in neural networks. Crucially, Tanaka’s large- $N$  analysis shows the resulting HCIZ  
 3496 exponent depends only on the eigenvalue spectrum, so the final integrated- $R$  expression should  
 3497 remain applicable even when full rotational invariance is later broken in training.

Using a source matrix  $\mathbf{D}$  to represent  $d\mu(\mathbf{A})$  with  $d\mu(\mathbf{W})$ . We consider all matrices  $\mathbf{A}$  with the same limiting spectral density,  $\rho_{\mathbf{A}}^{\infty}(\lambda)$ , as the limiting (*empirical*) ESD of the Teacher. That is, we want  $\rho_{\mathbf{A}}^{\infty}(\lambda) = \rho_{\mathbf{W}}^{\infty}(\lambda)$ , where  $\mathbf{T} = \mathbf{W}$ . Of course, there are infinitely many weight matrices  $\mathbf{W}$  with the same  $M$  eigenvalues,  $\{\lambda_i\}_{i=1}^M$ , as the Teacher. Let us specify these matrices with the measure  $d\mu(\mathbf{W})$ . Doing this lets us then write the measure  $d\mu(\mathbf{A})$  in terms of  $d\mu(\mathbf{W})$  as:

$$d\mu(\mathbf{A}) := e^{-\frac{n\beta}{2}\text{Tr}[\mathbf{W}\mathbf{D}\mathbf{W}^{\top}]}d\mu(\mathbf{W}), \quad (256)$$

where  $\mathbf{D}$  is some  $M \times M$  matrix, called the Source Matrix, to be specified below, and the  $\frac{1}{2}$  here as well. Indeed, the key idea here will be to define  $\mathbf{D}$  in such a way as to obtain the desired final result. Notice also that we have added an  $n\beta$  term; this will be factored out later.

We can now represent the partition function  $\mathbb{Z}^{IZ}$ , by inserting Eqn. 256 into Eqn. 253.  $\mathbb{Z}^{IZ}$  is now defined as an integral over all possible (Teacher) weight matrices  $\mathbf{W}$

$$\mathbb{Z}^{IZ} = \int d\mu(\mathbf{W}) \exp \left[ \frac{n\beta}{2} (\text{Tr}[\mathbf{W}^{\top} \mathbf{A}_N \mathbf{W}] - \text{Tr}[\mathbf{W}\mathbf{D}\mathbf{W}^{\top}]) \right], \quad (257)$$

Observe that this integral only converges when all the eigenvalues of  $\mathbf{D}$ ,  $\{\vartheta_{\mu}\}_{\mu=1}^M$ , are larger than the maximum eigenvalue of  $\mathbf{A}$ , i.e., when  $\vartheta_{\mu} > \lambda_{max}$ , for  $\mu \in [1, M]$  (although below this will become  $n\beta\vartheta_{\mu} > \lambda_{max}$ ). Later, we will place  $\mathbf{D}$  in diagonal form, and we will obtain an explicit expression for its  $M$  eigenvalues in terms of the  $M$  non-zero eigenvalues of  $\mathbf{X}$ . The eigenvalues of  $\mathbf{D}$  will turn out to Lagrange Multipliers, needed later.

### The Saddle Point Approximation (SPA) and the Large Deviation Principle (LDP).

To evaluate the large- $N$  case of  $\beta\Gamma_{\tilde{Q}^2}^{IZ}$  (see 254, 255), we assume that the distribution of possible Teacher correlation matrices,  $\mu(\mathbf{X})$ , satisfies a *Large Deviation Principle (LDP)*. An LDP applies to probability distributions that take an exponential form, such that  $\mu(\mathbf{X}) = e^{-NI(\mathbf{X})}d\mu(\mathbf{X})$ , where  $I(\mathbf{X})$  is Entropy or Rate function  $I(\mathbf{X})$ .

In applying an LDP, we effectively restrict measure of student correlation matrices  $\mathbf{A}$  to those most similar to the empirically observed Teacher correlation matrix  $\mathbf{X}$ . We expect the measure over all Teacher correlation matrices follows an LDP because the ESD is far from Gaussian, the dominant generalizing components reside in the tail of the ESD, and at finite-size the tail decays at worst as an exponentially Truncated Power Law (TPL).

**Three 3 steps to evaluate  $\langle \mathbb{Z}^{IZ} \rangle_{\mathbf{A}}$  in the Wide Layer large- $N$  approximation.** The goal is to start with Eqn. 257 and obtain two separate, equivalent relations, Eqns. 258 and 260:

1. **Obtaining an integral transform of  $\rho_{\mathbf{A}}^{\infty}(\lambda)$ .** First, we expand and reduce Eqn. 257 and evaluate the expected value of  $\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}] = \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}]$  in the Large- $\mathcal{N}$  limit in  $N$  by expressing the  $\rho_{\mathbf{A}}(\lambda)$  for the  $N \times N$  matrix  $\mathbf{A} = \mathbf{A}_N = \frac{1}{N}\mathbf{S}\mathbf{S}^{\top}$  in the continuum representation, i.e., as  $\rho_{\mathbf{A}}^{emp}(\lambda) \rightarrow \rho_{\mathbf{A}}^{\infty}(\lambda)$ , to obtain:

$$\lim_{N \gg 1} \frac{1}{N} \ln \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] = M \ln \left( \frac{2\pi}{n\beta} \right) - \sum_{\mu=1}^M \int \ln(\delta_{\mu} - \lambda) \rho_{\mathbf{A}}^{\infty}(\lambda) d\lambda. \quad (258)$$

This gives us an  $\mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}]$  in terms of an integral transform  $\rho_{\mathbf{A}}^{\infty}(\lambda)$ , which we can model.<sup>48</sup>

<sup>48</sup>This integral of  $\rho_{\mathbf{A}}^{\infty}(\lambda)$  is related to the *Shannon Transform*, an integral transform from information theory that is useful when analyzing the mutual information or the capacity of a communication channel [83].

3531 **2. Forming the Saddle Point Approximation (SPA).** We evaluate Eqn. 257 as the ex-  
 3532 pected value of  $\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}] = \mathbb{E}_{\mathbf{A}_M}[\mathbb{Z}^{IZ}]$  for the  $M \times M$  matrix  $\mathbf{A} = \mathbf{A}_M = \frac{1}{N} \mathbf{S}^\top \mathbf{S}$  (but explicitly  
 3533 in terms of  $d\mu(\mathbf{X})$ ). Then, taking in the large- $N$  approximation using the SPA, (and which  
 3534 can be done implicitly using the LDP), we obtain

$$\lim_{N \gg 1} \mathbb{E}_{\mathbf{A}_M}[\mathbb{Z}^{IZ}] \simeq \int \exp(n\beta N \text{Tr}[\mathcal{G}(\mathbf{X})]) d\mu(\mathbf{X}) \approx \exp(n\beta N \mathcal{G}^{max}) \quad (259)$$

3535 where  $\mathcal{G}(\mathbf{X})$  depends on  $\mathbb{G}_{\mathbf{A}}(\mathbf{X})$ , and  $\mathcal{G}^{max} = \sup_{\mathbf{X}} \mathcal{G}(\mathbf{X})$ . We can then write

$$\lim_{N \gg 1} \frac{1}{N} \ln \mathbb{E}_{\mathbf{A}_M}[\mathbb{Z}^{IZ}] \approx n\beta \mathcal{G}^{max}, \quad (260)$$

3536 **3. Finding the Inverse Legendre Transform.** To do this, we now equate

$$\lim_{N \gg 1} \frac{1}{N} \ln \mathbb{E}_{\mathbf{A}_M}[\mathbb{Z}^{IZ}] = \lim_{N \gg 1} \frac{1}{N} \ln \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] \quad (261)$$

3537 Then, we can form the inverse Legendre transform which we will let us relate  $\mathbb{G}_{\mathbf{A}}(\lambda)$  in  
 3538 Eqn. 251 to the integrated R-transform of  $\rho_{\mathbf{A}}^\infty(\lambda)$ .

3539 (See A.6.4.)

#### 3540 **A.6.2 Step 1. Forming the Integral Transformation of ESD ( $\rho_{\mathbf{A}}^\infty(\lambda)$ )**

3541 We first establish Eqn. 258, in Steps 1.1 – 1.4. This is done by changing variables under a Unitary  
 3542 transformation,  $\mathbf{W} \rightarrow \check{\mathbf{W}}$ , evaluating the resulting functional determinant, and then taking the  
 3543 continuum limit of the ESD  $\tilde{\rho}_{\mathbf{A}}(\lambda) \rightarrow \rho_{\mathbf{A}}^\infty(\lambda)$ .

3544 **Step 1.1** To do so, let us first assume that Teacher correlation matrix  $\mathbf{X}$  and the source matrix  
 3545  $\mathbf{D}$  are simultaneously diagonalizable (i.e., their commutator is zero:  $[\mathbf{X}, \mathbf{D}] = 0$ ). In this case, we  
 3546 may write the generating function  $\mathbb{Z}^{IZ}$  in Eqn. 257 as

$$\mathbb{Z}^{IZ} = \int d\mu(\mathbf{W}) \exp \frac{n\beta}{2} \left( \text{Tr}[\mathbf{W}^\top \mathbf{U}^\top \mathbf{A} \mathbf{U} \mathbf{W}] - \text{Tr}[\mathbf{W} \mathbf{V}^\top \mathbf{\Delta} \mathbf{V} \mathbf{W}^\top] \right), \quad (262)$$

3547 where we have defined

$$\mathbf{A}_N = \mathbf{U}^\top \mathbf{A} \mathbf{U}, \quad \mathbf{D} = \mathbf{V}^\top \mathbf{\Delta} \mathbf{V}, \quad (263)$$

3548 where  $\mathbf{U}$  ( $N \times N$ ) and  $\mathbf{V}$  ( $M \times M$ ) are Unitary matrices. Since  $\mathbf{U}^\top \mathbf{U} = \mathbf{I}$  and  $\mathbf{V}^\top \mathbf{V} = \mathbf{I}$ , we can  
 3549 insert these identities into  $\mathbb{Z}^{IZ}$  in 262, giving

$$\mathbb{Z}^{IZ} = \int d\mu(\mathbf{W}) \exp \frac{n\beta}{2} \times \left( \text{Tr}[(\mathbf{V}^\top \mathbf{V}) \mathbf{W}^\top \mathbf{U}^\top \mathbf{A} \mathbf{U} \mathbf{W} (\mathbf{V}^\top \mathbf{V})] - \text{Tr}[(\mathbf{U}^\top \mathbf{U}) \mathbf{W} \mathbf{V}^\top \mathbf{\Delta} \mathbf{V} \mathbf{W}^\top (\mathbf{U}^\top \mathbf{U})] \right). \quad (264)$$

3550 We can identify the reduced weight matrix  $\check{\mathbf{W}}$  as

$$\check{\mathbf{W}} = \mathbf{U} \mathbf{W} \mathbf{V}^\top, \quad \check{\mathbf{W}}^\top = \mathbf{V} \mathbf{W}^\top \mathbf{U}^\top, \quad (265)$$

3551 Rearranging parentheses, this gives

$$\mathbb{Z}^{IZ} = \int d\mu(\mathbf{W}) \exp \frac{n\beta}{2} \times \left( \text{Tr}[\mathbf{V}^T (\mathbf{V} \mathbf{W}^T \mathbf{U}^T) \mathbf{A} (\mathbf{U} \mathbf{W} \mathbf{V}^T) \mathbf{V}] - \text{Tr}[\mathbf{U}^\top (\mathbf{U} \mathbf{W} \mathbf{V}^\top) \mathbf{\Delta} (\mathbf{V} \mathbf{W}^\top \mathbf{U}^\top) \mathbf{U}] \right). \quad (266)$$

3552 We can now express  $\mathbb{Z}^{IZ}$  in terms of  $\check{\mathbf{W}}$  as

$$\mathbb{Z}^{IZ} = \int d\mu(\mathbf{W}) \exp \frac{n\beta}{2} \left( \text{Tr}[\mathbf{V}^\top \check{\mathbf{W}}^\top \mathbf{\Lambda} \check{\mathbf{W}} \mathbf{V}] - \text{Tr}[\mathbf{U}^\top \check{\mathbf{W}} \mathbf{\Delta} \check{\mathbf{W}}^\top \mathbf{U}] \right). \quad (267)$$

3553 Since the Trace operator  $\text{Tr}[\cdot]$  is invariant to Unitary (Orthogonal) transformations, we can now  
 3554 remove the  $\mathbf{U}$  and  $\mathbf{V}$  terms, giving the simplified expression for our generating function  $\mathbb{Z}^{IZ}$  in  
 3555 terms of the two diagonal matrices  $\mathbf{\Lambda}, \mathbf{\Delta}$ , the reduced weight matrix  $\check{\mathbf{W}}$ , and the Jacobian  $J(\check{\mathbf{W}})$   
 3556 transformation for  $d\mu(\mathbf{W}) \rightarrow d\mu(\check{\mathbf{W}})$ , as:

$$\mathbb{Z}^{IZ} = \int d\mu(\check{\mathbf{W}}) J(\check{\mathbf{W}}) \exp \frac{n\beta}{2} \left( \text{Tr}[\check{\mathbf{W}}^\top \mathbf{\Lambda} \check{\mathbf{W}}] - \text{Tr}[\check{\mathbf{W}} \mathbf{\Delta} \check{\mathbf{W}}^\top] \right). \quad (268)$$

3557 **Step 1.2** We can now evaluate the integral using the standard relation for the functional de-  
 3558 terminant for infinite-dimensional Gaussian integrals [102]

$$\mathbb{Z}^{IZ} = \left( \frac{2\pi}{n\beta} \right)^{NM/2} \det(\mathbf{\Delta} - \mathbf{\Lambda})^{-1/2} \quad (269)$$

3559 where the Jacobian is unity for the Unitary transformation.

$$J(\check{\mathbf{W}}) = 1. \quad (270)$$

3560 since  $\mathbf{W} \mapsto \check{\mathbf{W}}$  is an orthogonal transformation. We now use the standard Trace-Log-Determinant  
 3561 relation [102]

$$\text{Tr}[\ln \mathbf{M}] = \ln \det \mathbf{M}. \quad (271)$$

3562 Let us insert  $(\exp \ln)$  on the R.H.S. of 269, to obtain

$$\begin{aligned} \mathbb{Z}^{IZ} &= \exp \ln \left[ \left( \frac{2\pi}{n\beta} \right)^{NM/2} \det(\mathbf{\Delta} - \mathbf{\Lambda})^{-1/2} \right] \\ &= \exp \left[ \left( \frac{NM}{2} \right) \ln \frac{2\pi}{n\beta} - \frac{1}{2} \text{Tr}[\ln(\mathbf{\Delta} - \mathbf{\Lambda})] \right] \\ &= \exp \left[ \frac{NM}{2} \ln \frac{2\pi}{n\beta} - \frac{1}{2} \ln \det(\mathbf{\Delta} - \mathbf{\Lambda}) \right]. \end{aligned} \quad (272)$$

3563 **Step 1.3** We now want to express the generating function  $\mathbb{Z}^{IZ}$  in 272 in terms of an integral  
 3564 over the continuous limiting spectral density  $\rho_{\mathbf{A}}(\lambda)$  of the correlation matrix  $\mathbf{A}_N$ .

3565 First, we express the Determinant of the matrix  $\mathbf{\Delta} - \mathbf{\Lambda}$  in terms of discrete eigenvalues:

$$\det(\mathbf{\Delta} - \mathbf{\Lambda})^{-1/2} = \prod_{\mu=1}^M \prod_{i=1}^N (\vartheta_\mu - \lambda_i)^{-1/2}. \quad (273)$$

3566 This gives the Log-Determinant in terms of the  $M$  (non-zero) eigenvalues of  $\mathbf{D}$  and  $\mathbf{A}_N$ , as

$$\ln \det(\mathbf{\Delta} - \mathbf{\Lambda})^{-1/2} = -\frac{1}{2} \sum_{\mu=1}^M \sum_{i=1}^N \ln(\vartheta_\mu - \lambda_i). \quad (274)$$

3567 We can express the ESD,  $\tilde{\rho}_{\mathbf{A}}(\lambda)$ , of the Student Correlation matrix  $\mathbf{A}_N$  in terms of the Dirac  
 3568 delta-function,  $\delta(x)$ , as

$$\tilde{\rho}_{\mathbf{A}}(\lambda) = \frac{1}{N} \sum_{i=1}^N \delta(\lambda - \lambda_i). \quad (275)$$



Using this, the Expected Value of the Log-Determinant in 274 can be expressed in terms of the ESD of  $\mathbf{A}_N$  as

$$\begin{aligned}\langle \ln \det (\mathbf{\Delta} - \mathbf{\Lambda})^{-1/2} \rangle_{\mathbf{A}_N} &= -\frac{1}{2} \sum_{\mu=1}^M \sum_{i=1}^N \int d\lambda \ln(\vartheta_\mu - \lambda) \delta(\lambda - \lambda_i) \\ &= -\frac{1}{2} \sum_{\mu=1}^M \int d\lambda \ln(\vartheta_\mu - \lambda) \sum_{i=1}^N \delta(\lambda - \lambda_i) \\ &= -\frac{1}{2} \sum_{\mu=1}^M \int d\lambda \ln(\vartheta_\mu - \lambda) N \tilde{\rho}_{\mathbf{A}}(\lambda).\end{aligned}\quad (276)$$

Let us insert this back into our expression for the generating function, 272, giving  $\mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}]$  in terms of the ESD  $\tilde{\rho}_{\mathbf{A}}$  as

$$\mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] = \exp \left\{ \frac{N}{2} \left[ M \ln \frac{2\pi}{n\beta} - \sum_{\mu=1}^M \int d\lambda \ln(\vartheta_\mu - \lambda) \tilde{\rho}_{\mathbf{A}}(\lambda) \right] \right\}. \quad (277)$$

We can now replace the sum over the  $N$  eigenvalues  $\lambda_i$  with an integral over the limiting ESD,  $\rho(\lambda)$ , to obtain

$$\rho_{\mathbf{A}}^\infty(\lambda) = \lim_{N \rightarrow \infty} \tilde{\rho}_{\mathbf{A}}(\lambda). \quad (278)$$

Observe that this effectively means that we are taking a Large- $\mathcal{N}$  limit in  $N$ ,  $N \gg 1$ . This lets us write the Expected Value of the generating function  $\mathbb{Z}^{IZ}$  in 277 as

$$\lim_{N \gg 1} \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] = \exp \left\{ \frac{N}{2} \left[ M \ln \frac{2\pi}{n\beta} - \sum_{\mu=1}^M \int d\lambda \ln(\vartheta_\mu - \lambda) \rho_{\mathbf{A}}^\infty(\lambda) \right] \right\} \quad (279)$$

**Step 1.4** Using the Self-Averaging Property,

$$\ln \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] \simeq \langle \ln \mathbb{Z}^{IZ} \rangle_{\mathbf{A}_M}, \quad (280)$$

It follows from Eqn. 279 that

$$\lim_{N \gg 1} \ln \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] \simeq \frac{NM}{2} \ln \frac{2\pi}{n\beta} - \frac{N}{2} \sum_{\mu=1}^M \int d\lambda \ln(\vartheta_\mu - \lambda) \rho_{\mathbf{A}}^\infty(\lambda). \quad (281)$$

The  $N$ -dependence now cancels out, and we are left an approximate expression due to the remaining dependence of the continuum limiting density  $\rho_{\mathbf{A}}^\infty(\lambda)$  (for  $\mathbf{A} = \mathbf{A}_N$ )

$$\lim_{N \gg 1} \frac{2}{N} \ln \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] = M \ln \frac{2\pi}{n\beta} - \sum_{\mu=1}^M \int d\lambda \ln(\vartheta_\mu - \lambda) \rho_{\mathbf{A}}^\infty(\lambda). \quad (282)$$

This completes the derivation of Eqn. 258; we have an expression for the expected value of  $\mathbb{Z}^{IZ}$ , evaluated in the Large- $\mathcal{N}$  (continuum) limit in  $N$ .

### A.6.3 Step 2: The Saddle Point Approximation (SPA): Explicitly forming the Large Deviation Principle (LDP)

We now evaluate  $\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}]$  in Eqn. 259 as  $\mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}]$  to establish Eqn. 260, .

Using the LDP (and following similar approaches in spin glass theory [96]), below we will show that we can write the expected value of  $\mathbb{Z}^{IZ}$  in terms of  $d\mu(\mathbf{X})$  now (which is equivalent to  $d\mu(\mathbf{A}_M)$ ) and in the large- $N$  approximation, as

$$\lim_{N \gg 1} \mathbb{E}_{\mathbf{A}_M}[\mathbb{Z}^{IZ}] = \int \exp(n\beta N \text{Tr}[\mathbb{G}_{\mathbf{A}}(\mathbf{X})] - NI(\mathbf{X}) + o(N)) d\mu(\mathbf{X}) \quad (283)$$

where  $I(\mathbf{X})$  is Rate Function, defined below, and  $\mathbb{G}_{\mathbf{A}}(\mathbf{X})$  is what we are eventually solving for.

3590 **Step 2.0** We start with the *expected* Partition Function

$$\mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}] = \int d\mu(\mathbf{A}) \int d\mu(\mathbf{W}) \exp\left[\frac{n\beta}{2} \text{Tr}[\mathbf{W}^\top \mathbf{A}_N \mathbf{W}] - \frac{n\beta}{2} \text{Tr}[\mathbf{W} \mathbf{D} \mathbf{W}^\top]\right]. \quad (284)$$

3591 The average over  $\mathbf{A}_N$  affects only the first exponential; applying the SPA, we **define** a matrix  
3592 function  $\mathcal{G}(\mathbf{X})$ , depending solely on  $\mathbf{X} = \frac{1}{N} \mathbf{W}^\top \mathbf{W}$ , by

$$\int d\mu(\mathbf{A}) \exp\left[\frac{n\beta}{2} \text{Tr}[\mathbf{W}^\top \mathbf{A}_N \mathbf{W}]\right] = \exp\left[\frac{n\beta N}{2} \text{Tr}[\mathcal{G}(\mathbf{X})]\right]. \quad (285)$$

3593 which will be valid in the large- $N$  in  $N$  approximation below.

3594 We now note that given the duality of measures, we can assert

$$\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}] = \mathbb{E}_{\mathbf{A}_M}[\mathbb{Z}^{IZ}] = \mathbb{E}_{\mathbf{A}_N}[\mathbb{Z}^{IZ}]. \quad (286)$$

3595 This lets us insert (285) into (284) and then write

$$\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}] = \int d\mu(\mathbf{W}) \exp\left[\frac{n\beta N}{2} \text{Tr}[\mathcal{G}(\mathbf{X})] - \frac{n\beta}{2} \text{Tr}[\mathbf{W} \mathbf{D} \mathbf{W}^\top]\right]. \quad (287)$$

3596 The now need to determine an explicit form for  $\mathcal{G}(\mathbf{X})$ . We introduce a new change of measure,  
3597  $d\mu(\mathbf{W}) \rightarrow d\mu(\mathbf{X})$ . Then, we show this lets us express  $\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}]$  as  $\mathbb{E}_{\mathbf{X}}[\mathbb{Z}^{IZ}]$  and to express it using  
3598 the LDP. Next, we apply a SPA to solve for  $\mathcal{G}^{max} = \max \mathbb{G}_{\mathbf{A}}$ . Importantly, we also show how to  
3599 incorporate the inverse-Temperature  $n\beta$ , which is new.

3600 **Step 2.1** To define the transformation  $d\mu(\mathbf{W}) \rightarrow d\mu(\mathbf{X})$ , where (recall)  $\mathbf{X} = \frac{1}{N} \mathbf{W}^\top \mathbf{W}$ , we use  
3601 the (again) the integral representation of the Dirac delta-function  $\delta(x)$ :

$$\delta(x) := \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\hat{x}x} d\hat{x}. \quad (288)$$

3602 This lets us express the transformation of measure  $d\mu(\mathbf{W}) \rightarrow d\mu(\mathbf{X})$  (approximately) as

$$\begin{aligned} d\mu(\mathbf{W}) &:= \delta\left(\frac{1}{2} \text{Tr}[N\mathbf{X} - \mathbf{W}^\top \mathbf{W}]\right) d\mu(\mathbf{X}) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\frac{1}{2} \text{Tr}[\hat{X}(N\mathbf{X} - \mathbf{W}^\top \mathbf{W})]} d\mu(\mathbf{X}) d\mu(\hat{X}), \end{aligned} \quad (289)$$

3603 where  $\hat{X}$  is a scalar (or really a matrix of scalars), and we have  $\frac{1}{2}$  term for mathematical consis-  
3604 tency below. <sup>49</sup>

3605 **Step 2.2** Next, we take a Wick Rotation<sup>50</sup>,  $i\hat{X} \rightarrow -\hat{X}$ , so that the terms under the integral are  
3606 all real (not complex), giving:

$$d\mu(\mathbf{W}) = \mathcal{N}_{Wick} \int_{-i\infty}^{i\infty} e^{\frac{1}{2} \text{Tr}[\hat{X}(N\mathbf{X} - \mathbf{W}^\top \mathbf{W})]} d\mu(\mathbf{X}) d\mu(\hat{X}). \quad (290)$$

3607 where  $d\mu(\hat{X})$  is a measure over  $\frac{M(M-1)}{2}$  Lagrange multipliers, and the normalization is

$$\mathcal{N}_{Wick} = \left(\frac{1}{2\pi i}\right)^{\frac{M(M-1)}{2}} \quad (291)$$

<sup>49</sup>The full change of measure would require a delta function constraint for each matrix element  $X_{i,j}$ , i.e.,  $\delta\left(\frac{1}{2}N(X_{i,j} - [\mathbf{W}^\top \mathbf{W}]_{i,j})\right)$ . Here, we assume the Trace constraint is sufficient for our level of rigor.

<sup>50</sup>The Wick rotation converts an oscillatory integral into an exponentially decaying one which should be well defined. Technically, this is an analytic continuation which needs to be checked, but following standard practice in physics we will assume the resulting integral is analytic and therefore well defined and we will proceed onward.

3608 **Step 2.3** We now insert 290 into 287, which lets us express  $\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}]$  as an integral over the  
 3609 Teacher Correlation matrices.

$$\begin{aligned}\mathbb{E}_{\mathbf{A}}[\mathbb{Z}^{IZ}] &= \mathcal{N}_{Wick} \int_{\mathbf{X}} \int_{-i\infty}^{i\infty} e^{N \frac{n\beta}{2} \text{Tr}[\mathcal{G}(\mathbf{X})] + \frac{N}{2} \text{Tr}[\hat{X}\mathbf{X}]} e^{-\frac{1}{2} \text{Tr}[\hat{X}\mathbf{W}^\top \mathbf{W}]} e^{\frac{n\beta}{2} \text{Tr}[\mathbf{W}\mathbf{D}\mathbf{W}^\top]} d\mu(\hat{X}) d\mu(\mathbf{X}) \\ &= \mathcal{N}_{Wick} \int_{\mathbf{X}} \int_{-i\infty}^{i\infty} e^{N \frac{n\beta}{2} \text{Tr}[\mathcal{G}(\mathbf{X})] + \frac{N}{2} \text{Tr}[\hat{X}\mathbf{X}]} e^{-\frac{1}{2} \text{Tr}[\mathbf{W}\hat{X}\mathbf{W}^\top] + \frac{n\beta}{2} \text{Tr}[\mathbf{W}\mathbf{D}\mathbf{W}^\top]} d\mu(\hat{X}) d\mu(\mathbf{X}) \\ &= \mathcal{N}_{Wick} \int_{\mathbf{X}} \int_{-i\infty}^{i\infty} e^{N \frac{n\beta}{2} \text{Tr}[\mathcal{G}(\mathbf{X})] + \frac{N}{2} \text{Tr}[\hat{X}\mathbf{X}]} e^{\frac{1}{2} \text{Tr}[\mathbf{W}(n\beta\mathbf{D} - \hat{X})\mathbf{W}^\top]} d\mu(\hat{X}) d\mu(\mathbf{X}).\end{aligned}\quad (292)$$

3610 **Step 2.4** We can now rearrange terms to make this expression look like the Eqn. 283 In Large  
 3611 Deviations Theory, the Rate Function is defined by the Legendre Transform,

$$\mathcal{I}(\mathbf{X}) = \sup_{\check{\mathbf{X}}} \left[ \text{Tr} \frac{1}{2} \mathbf{X}^\top \check{\mathbf{X}} - \ln \mathbb{M}(\check{\mathbf{X}}) \right], \quad (293)$$

3612 where  $\mathbb{M}(\check{\mathbf{X}})$  is the Moment Generating Function,  $\ln \mathbb{M}(\check{\mathbf{X}})$ , is the Cumulant Generating Function,  
 3613 and  $\check{\mathbf{X}}$  is a (matrix of) *Lagrange Multiplier*(s).  $\mathbb{M}(\check{\mathbf{X}})$  is defined in terms of the (unnormalized)  
 3614 density  $p(\mathbf{x})$  as

$$\mathbb{M}(\check{\mathbf{X}}) = \int \exp \left( \frac{1}{2} \mathbf{x}^\top \check{\mathbf{X}} \mathbf{x} \right) p(\mathbf{x}) d\mathbf{x} \quad (294)$$

3615 which, in turn, is defined in terms of the source matrix  $\mathbf{D}$ ,

$$p(\mathbf{x}) = \exp \left( -\frac{1}{2} \mathbf{x}^\top n\beta\mathbf{D}\mathbf{x} \right). \quad (295)$$

3616 The moment generating function  $\mathbb{M}(\check{\mathbf{X}})$  is then given by

$$\mathbb{M}(\check{\mathbf{X}}) = \int \exp \left( -\frac{1}{2} \mathbf{x}^\top (n\beta\mathbf{D} - \check{\mathbf{X}}) \mathbf{x} \right) d\mathbf{x} = (2\pi)^{\frac{M}{2}} \det(n\beta\mathbf{D} - \check{\mathbf{X}})^{-\frac{1}{2}}. \quad (296)$$

3617 **Step 2.5** The Saddle Point Approximation (SPA) can be used to solve for  $\mathcal{I}(\check{\mathbf{X}})$  by solving for  
 3618 the stationary conditions

$$\frac{\partial}{\partial \check{\mathbf{X}}} \mathcal{I}(\mathbf{X}, \check{\mathbf{X}}) = 0. \quad (297)$$

3619 First, let us compute  $\ln \mathbb{M}(\check{\mathbf{X}})$  as:

$$\ln \mathbb{M}(\check{\mathbf{X}}) = \frac{M}{2} \ln(2\pi) - \frac{1}{2} \ln \det(n\beta\mathbf{D} - \check{\mathbf{X}}). \quad (298)$$

3620 Substituting this into the expression for the Legendre transform, we obtain:

$$\mathcal{I}(\mathbf{X}, \check{\mathbf{X}}) = \sup_{\check{\mathbf{X}}} \left[ \frac{1}{2} \text{Tr}[\mathbf{X}\check{\mathbf{X}}] - \frac{M}{2} \ln(2\pi) + \frac{1}{2} \ln \det(n\beta\mathbf{D} - \check{\mathbf{X}}) \right]. \quad (299)$$

3621 The supremum of this expression is attained at the value of  $\check{\mathbf{X}}$  that satisfies:

$$\frac{\partial}{\partial \check{\mathbf{X}}} \left[ \frac{1}{2} \text{Tr}[\mathbf{X}\check{\mathbf{X}}] + \frac{1}{2} \ln \det(n\beta\mathbf{D} - \check{\mathbf{X}}) \right] = 0. \quad (300)$$

3622 Taking the derivative, we obtain

$$\frac{1}{2} \mathbf{X} + \frac{1}{2} (n\beta\mathbf{D} - \check{\mathbf{X}})^{-1} = 0, \quad (301)$$

3623 which simplifies to:

$$\mathbf{X} = (n\beta\mathbf{D} - \check{\mathbf{X}})^{-1} \Rightarrow \check{\mathbf{X}} = n\beta\mathbf{D} - \mathbf{X}^{-1}. \quad (302)$$

3624 Substituting  $\check{\mathbf{X}} = n\beta\mathbf{D} - \mathbf{X}^{-1}$  back into the expression for  $I(\mathbf{X})$ , we obtain:

$$I(\mathbf{X}) = \frac{1}{2} \left[ \text{Tr} [\mathbf{X}(n\beta\mathbf{D} - \mathbf{X}^{-1})] - \frac{M}{2} \ln(2\pi) + \frac{1}{2} \ln \det (\mathbf{X}^{-1}) \right]. \quad (303)$$

3625

$$\text{Tr} [\mathbf{X}n\beta\mathbf{D} - \mathbf{I}] = \text{Tr} [\mathbf{X}n\beta\mathbf{D}] - N, \quad (304)$$

3626

$$\ln \det (\mathbf{X}^{-1}) = -\ln \det (\mathbf{X}), \quad (305)$$

3627 we get:

$$I(\mathbf{X}) = \frac{1}{2} [\text{Tr} [\mathbf{X}n\beta\mathbf{D}] - \ln \det (\mathbf{X}) - M - M \ln(2\pi)]. \quad (306)$$

3628 Finally, we express  $I(\mathbf{X})$  in the form:

$$I(\mathbf{X}) = \frac{1}{2} [-M(1 + \ln(2\pi)) + \text{Tr} [\mathbf{X}n\beta\mathbf{D}] - \ln \det (\mathbf{X})]. \quad (307)$$

## Step 2.6

$$n\beta\mathcal{G}(\mathbf{X}) = M(1 + \ln 2\pi) + n\beta \text{Tr} [\mathbb{G}_{\mathbf{A}}(\mathbf{X})] - \text{Tr} [\mathbf{X}n\beta\mathbf{D}] + \ln \det (\mathbf{X}). \quad (308)$$

3629 We restrict our solution to those where  $\mathbf{X}$  and  $n\beta\mathbf{D}$  can be diagonalized simultaneously. In  
3630 particular, this lets us write

$$\text{Tr} [\mathbf{X}n\beta\mathbf{D}] = \sum_{\mu=1}^M n\beta\delta_{\mu}\lambda_{\mu}, \quad (309)$$

3631 where  $n\beta\delta_{\mu}$  and  $\lambda_{\mu}$  denote the eigenvalues of  $\mathbf{X}$  and  $n\beta\mathbf{D}$ , resp.

3632 We can now write the maximum value of  $\mathbb{G}_{\mathbf{A}}$ ,  $\mathcal{G}^{max}$ , as

$$n\beta\mathcal{G}^{max} = M \left( 1 + \ln \frac{2\pi}{n\beta} \right) - \sum_{\mu=1}^M \min_{n\beta\delta_{\mu}} [n\beta\delta_{\mu}\lambda_{\mu} - n\beta\mathbb{G}_{\mathbf{A}}(\lambda_{\mu}) + \ln \lambda_{\mu}]. \quad (310)$$

## A.6.4 Expressing the Norm Generating Function ( $\mathbb{G}_{\mathbf{A}}(\lambda)$ ) as the Integrated R-transform ( $R(z)$ ) of the Correlation Matrix ( $\mathbf{A}$ )

3633 Having completed both steps, let us combine Eqns. 258, 282 with 260 and 310. We follow the  
3636 first arguments by Tanaka [83] (which follows Cherrier [134]).

$$M \ln \left( \frac{2\pi}{n\beta} \right) - \sum_{\mu=1}^M \int \ln(n\beta\delta_{\mu} - \lambda) \rho_{\mathbf{A}}^{\infty}(\lambda) d\lambda = M \left( 1 + \ln \frac{2\pi}{n\beta} \right) - \sum_{\mu=1}^M \min_{n\beta\delta_{\mu}} [n\beta\delta_{\mu}\lambda_{\mu} - n\beta\mathbb{G}_{\mathbf{A}}(\lambda_{\mu}) + \ln \lambda_{\mu}]. \quad (311)$$

3637 By canceling the  $\ln \frac{2\pi}{n\beta}$  term from both sides, we obtain

$$- \sum_{\mu=1}^M \int \ln(n\beta\delta_{\mu} - \lambda) \rho_{\mathbf{A}}^{\infty}(\lambda) d\lambda = M - \sum_{\mu=1}^M \min_{n\beta\delta_{\mu}} [n\beta\delta_{\mu}\lambda_{\mu} - n\beta\mathbb{G}_{\mathbf{A}}(\lambda_{\mu}) + \ln \lambda_{\mu}]. \quad (312)$$

3638 Since this is true for every  $\mu$ , we can solve this for any arbitrary eigenvalue  $\lambda_{\mu}$ .

3639 Dropping the  $\mu$  subscript, we have the following identity:

$$\min_{\delta} [n\beta\delta\lambda - n\beta\mathbb{G}_{\mathbf{A}}(\lambda) + \ln \lambda] = 1 - \int \ln(n\beta\delta - \lambda) \rho_{\mathbf{A}}^{\infty}(\lambda) d\lambda. \quad (313)$$

We need to invert 313 in order to find  $n\beta\mathbb{G}_{\mathbf{A}}(\lambda)$ . If we choose the eigenvalues of  $\mathbf{D}$  such that  $n\beta\delta_{\mu} > \lambda_{max}$  for all  $\mu$ , then this relation is concave and therefore invertible via a Legendre transform.

This gives

$$n\beta\mathbb{G}_{\mathbf{A}}(\lambda) = n\beta\delta(\lambda)\lambda - \int \ln[n\beta\delta(\lambda) - \lambda]\rho_{\mathbf{A}}^{\infty}(\lambda)d\lambda - \ln\lambda - 1, \quad (314)$$

where we need to define  $n\beta\delta(\lambda)$ , which (not to be confused with the Dirac delta-function), describes the functional dependence between the eigenvalues of the source matrix  $\mathbf{D}$  and the Student Correlation Matrix  $\mathbf{A}$ .

$\mathbb{G}_{\mathbf{A}}(\lambda)$  is computed by minimizing over  $\delta$ , ensuring the relationship holds for the entire spectrum. So let us take the derivative of  $n\beta\mathbb{G}_{\mathbf{A}}$  w.r.t.  $\lambda$ . Term by term, this gives:

$$\frac{d}{d\lambda} n\beta\delta(\lambda)\lambda = n\beta\delta(\lambda) + \frac{dn\beta\delta(\lambda)}{d\lambda}\lambda \quad (315)$$

$$\frac{d}{d\lambda} \ln\lambda = \frac{1}{\lambda} \quad (316)$$

$$\begin{aligned} \frac{d}{d\lambda} \int \ln[n\beta\delta(\lambda) - \lambda]\rho_{\mathbf{A}}^{\infty}(\lambda)d\lambda &= \int \frac{d}{d\lambda} \ln[n\beta\delta(\lambda) - \lambda]\rho_{\mathbf{A}}^{\infty}(\lambda)d\lambda \\ &= \int \frac{dn\beta\delta(\lambda)}{d\lambda} \frac{\rho_{\mathbf{A}}^{\infty}(\lambda)}{n\beta\delta(\lambda) - \lambda} d\lambda \\ &= \frac{dn\beta\delta(\lambda)}{d\lambda} \int \frac{\rho_{\mathbf{A}}^{\infty}(\lambda)}{n\beta\delta(\lambda) - \lambda} d\lambda \end{aligned} \quad (317)$$

We can now simplify by defining  $\delta(\lambda)$  implicitly by the integral relation

$$\lambda = \int \frac{\rho_{\mathbf{A}}^{\infty}(\lambda)}{n\beta\delta(\lambda) - \lambda} d\lambda. \quad (318)$$

Combining terms, this gives

$$\frac{dn\beta\mathbb{G}_{\mathbf{A}}(\lambda)}{d\lambda} = n\beta\delta(\lambda) - \frac{1}{\lambda}, \quad (319)$$

Inverting the derivative, we obtain an integral equation for  $n\beta\mathbb{G}_{\mathbf{A}}(\lambda)$

$$n\beta\mathbb{G}_{\mathbf{A}}(\lambda) = \int_0^{\lambda} \left( n\beta\delta(z) - \frac{1}{z} \right) dz. \quad (320)$$

Notice since  $n\beta\delta(\lambda) \approx \frac{1}{\lambda}$  for  $\lambda \ll 1$ , then as  $\mathbb{G}_{\mathbf{A}}(0) = 0$  and we set the lower integrand to 0 (for now). Even though Tanaka's original proof assumes an analytic continuation without branch cuts, a heavy-tailed spectrum merely shifts the lower limit of the  $R$ -transform integral, so the expression for  $n\beta\mathcal{G}(\lambda)$  continues to hold.

To further connect these to the  $R$ -transform  $R_{\mathbf{A}}(z)$ , we recall that the Cauchy-Stieltjes (or just Cauchy See 135) transform  $\mathcal{C}_{\mathbf{A}}(z)$  is given by:

$$\mathcal{C}_{\mathbf{A}}(z) = \int \frac{\rho_{\mathbf{A}}(\lambda)}{z - \lambda} d\lambda. \quad (321)$$

The relationship between the Cauchy transform and the  $R$ -transform is then expressed as:

$$\mathcal{C}_{\mathbf{A}}\left(R_{\mathbf{A}}(z) + \frac{1}{z}\right) = z, \quad (322)$$

3661 which implies:

$$n\beta\mathbb{G}_{\mathbf{A}}(\lambda) = \int_0^\lambda R_{\mathbf{A}}(z)dz. \quad (323)$$

3662 WLOG, as mentioned earlier, we can replace the lower bound on  $\lambda$  from  $0 \rightarrow \tilde{\lambda}_{min}$  to obtain

$$n\beta\mathbb{G}_{\mathbf{A}}(\lambda) = \int_{\tilde{\lambda}_{min}}^\lambda \Re[R_{\tilde{\mathbf{A}}}(z)]dz. \quad (324)$$

3663 where  $\tilde{\lambda}_{min}$  corresponds to the start of the Effective Correlation Space (ECS), and, notably, take  
 3664 the *Real* part of  $R(z)$ . We take the Real part because the imaginary parts coming from the upper  
 3665 and lower lips of the cut cancel.<sup>51</sup>

## 3666 A.7 Existence of the Free $R$ -Transform for Power-Law Spectra

3667 In this subsection, we examine when the  $R$ -transform  $R(z)$  does and does not exist for power law  
 3668 tails.

### 3669 A.7.1 Analyticity criterion

3670 Recall the Cauchy–Stieltjes transform defined in Eq. (135) of Sec. 5.4.1,

$$G_\mu(z) = \int_{\mathbb{R}} \frac{\rho(\lambda)}{z - \lambda} d\lambda, \quad z \in \mathbb{C} \setminus \text{supp } \mu. \quad (325)$$

3671 If  $G_\mu(z)$  is *holomorphic* at  $z = \infty$  one may invert the map  $z = G_\mu(z)$  in a neighborhood of  $z = 0$   
 3672 and define

$$R_\mu(z) = G_\mu^{-1}(z) - \frac{1}{z}. \quad (326)$$

3673 Obstructions to the existence of  $R_\mu$  therefore coincide with non-analytic terms in the Laurent  
 3674 series of  $G_\mu$  about  $z = \infty$ . These can be easily removed, however, by considering that  $\rho(\lambda)$  is  
 3675 always strictly bounded from above by  $\lambda_{max}$ .

### 3676 A.7.2 Model and notation

3677 We first model a *bare* power-law tail regularized only by a hard lower cut-off  $\lambda_0 > 0$ :

$$\rho_\alpha(\lambda) = (\alpha - 1) \lambda_0^{\alpha-1} \lambda^{-\alpha}, \quad \lambda \geq \lambda_0, \quad \alpha \in \{2, 3, 4\}. \quad (327)$$

3678 Normalization is immediate:

$$\int_{\lambda_0}^\infty \rho_\alpha(\lambda) d\lambda = 1. \quad (328)$$

3679 The choice  $\alpha \in \{2, 3, 4\}$  mirrors the Heavy-Tailed exponents most frequently observed in  
 3680 neural-network weight and Hessian spectra.

---

<sup>51</sup>Alternatively, one might try to replace  $R(z)$  by its modulus; doing so breaks the Legendre relation  $G' = R$  and spoils the additivity of free cumulants.



### 3681 **A.7.3 Stieltjes (Green's) transform**

3682 For  $z \in \mathbb{C} \setminus [0, \infty)$

$$G_\alpha(z) = \int_{\lambda_0}^{\infty} \frac{\rho_\alpha(\lambda)}{z - \lambda} d\lambda. \quad (329)$$

3683 Carrying out the integration yields

$$G_{(2)}(z) = \frac{1}{z} + \frac{\lambda_0 \ln(1 - \frac{z}{\lambda_0})}{z^2}, \quad (330)$$

$$G_{(3)}(z) = \frac{1}{z} + \frac{2\lambda_0}{z^2} + \frac{2\lambda_0^2 \ln(1 - \frac{z}{\lambda_0})}{z^3}, \quad (331)$$

$$G_{(4)}(z) = \frac{1}{z} + \frac{3\lambda_0}{2z^2} + \frac{3\lambda_0^2}{z^3} + \frac{3\lambda_0^3 \ln(1 - \frac{z}{\lambda_0})}{z^4}. \quad (332)$$

3684 The logarithmic pieces carry the entire heavy-tail fingerprint; their placement in the expansion  
3685 dictates whether  $R(z)$  will be available.

### 3686 **A.7.4 Moments and free cumulants**

3687 Algebraic moments exist only up to order  $\alpha - 2$ :

$$m_k = \int_{\lambda_0}^{\infty} \lambda^k \rho_\alpha(\lambda) d\lambda = \frac{\alpha - 1}{\alpha - k - 1} \lambda_0^k, \quad k < \alpha - 1. \quad (333)$$

3688 Hence

$$m_1 = \frac{\alpha - 1}{\alpha - 2} \lambda_0, \quad m_2 = \frac{\alpha - 1}{\alpha - 3} \lambda_0^2 \quad (\alpha > 3). \quad (334)$$

3689 The first two free cumulants are  $\kappa_1 = m_1$  and  $\kappa_2 = m_2 - m_1^2$ .

### 3690 **A.7.5 R-transform for the bare tail**

3691 Define  $w = G_\alpha(z)$  and solve locally for  $R(z)$ . Using the finite cumulants one obtains

3692 •  $\alpha = 2$ : the logarithm appears at order  $z^{-2}$ ;  $G(z)$  is *not* analytic at infinity and the inversion  
3693 fails. *Conclusion: no R-transform. Truly  $1/\lambda^2$  tails are outside the remit of free addition.*

3694 •  $\alpha = 3$ :

$$R_{(3)}(z) = 2 \lambda_0 \quad (\text{constant}). \quad (335)$$

3695 Only a zeroth-order free cumulant survives, but that is *enough* for free convolution.

3696 •  $\alpha = 4$ :

$$R_{(4)}(z) = \frac{3}{2} \lambda_0 + \frac{3}{4} \lambda_0^2 w. \quad (336)$$

3697 Here the series truncates after the linear term; higher cumulants diverge.

3698 These three cases show explicitly how *incremental* changes in the tail exponent alter the  
3699 analytic status of  $G(z)$  and hence of  $R(z)$ . Since the higher-order free cumulants diverge, the  
3700 R-transform cannot be a finite polynomial. It must either be an infinite series (where the terms  
3701 beyond a certain point don't vanish) or, more strongly, exhibit non-analytic behavior (like the  
3702 logarithmic terms present in  $G(z)$ ) because its Taylor series coefficients (the cumulants) become  
3703 infinite. Fortunately,  $R(z)$  can be defined if we ensure that  $\rho(\lambda)$  has compact support.

### 3704 **A.7.6 Truncated $\alpha = 2$ power law**

3705 Introduce a cut-off  $\lambda_{max} > \lambda_0$  and set

$$\rho_{tr}(\lambda) = C \lambda^{-2}, \quad \lambda_0 \leq \lambda \leq \lambda_{max}, \quad C = \frac{1}{\lambda_0^{-1} - \lambda_{max}^{-1}}. \quad (337)$$

3706 Exact integration gives

$$G_{tr}(z) = C \left[ \frac{\log \lambda_{max} - \log(\lambda - z) - \log \lambda_0 + \log \lambda_0 - z}{z^2} - \frac{1}{\lambda_{max} z} + \frac{1}{\lambda_0 z} \right], \quad (338)$$

3707 valid for  $z \in \mathbb{C} \setminus [\lambda_0, \lambda_{max}]$ .

3708 **Expansion at  $z = \infty$ .** Using  $\log(\lambda - z) = \log z + \log(1 - \lambda_{max}/z)$  and  $\log(\lambda_0 - z) = \log z + \log(1 - \lambda_0/z)$ , the two  $\log z$  terms cancel and we find the regular series

$$G_{tr}(z) = \frac{1}{z} + \frac{m_1}{z^2} + \frac{m_2}{z^3} + \dots, \quad z \rightarrow \infty, \quad (339)$$

3710 with finite moments of all orders. Consequently

$$R_{tr}(z) = G_{tr}^{-1}(z) - \frac{1}{w} \quad (340)$$

3711 is analytic for  $|w|$  small.

3712 **Interpretation.** A truncation at any physically reasonable  $\lambda_{max}$ —for instance the largest  
3713 finite eigenvalue observed in a data set—instantly restores full analyticity at infinity. From the  
3714 point of view of free probability the system now behaves as if it had *all* moments, even though  
3715 the raw tail is still  $1/\lambda^2$  within  $[\lambda_0, \lambda_{max}]$ .

### 3716 **A.7.7 Key points and implications for SETOL**

- 3717 1. Cutting the tail at  $\lambda_{max} = \lambda_{max}^{ECS}$  *removes* the non-analytic  $\log z/z^2$  obstruction and turns  
3718 the free-probability machinery back on.
- 3719 2. Any model density  $\rho(\lambda)$  with compact support has  $G(z)$  analytic at  $z = \infty$ ; hence its  
3720  $R$ -transform equals the usual free-cumulant series and is available for algebraic manipula-  
3721 tion.
- 3722 3. In all theoretical derivations and numerical experiments in SETOL we therefore **model em-**  
3723 **pirical spectra as effectively as *truncated power laws*** (i.e with finite bounds, not  
3724 necessarily exponentially truncated). This choice is both empirically justified (no spectrum  
3725 is truly infinite) and mathematically essential: it guarantees that  $R(z)$  *always* exists.

### 3726 **A.7.8 Explicit $R$ -transforms for the truncated tail**

3727 We can also provide exact expressions for the leading terms (free cumulants) in  $R(z)$  for *alpha* =  
3728 2, 3, 4. The compact support  $[\lambda_0, \lambda_{max}] = [\tilde{\lambda}_{min}, \lambda_{max}^{ECS}]$  guarantees that every algebraic moment  
3729 (and free cumulant) is finite. Hence the Voiculescu series

$$R_{\alpha}^{tr}(z) = \sum_{n=1}^{\infty} \kappa_n z^{n-1}, \quad |z| \text{ small}, \quad (341)$$

converges for every  $\alpha > 1$ . Below we list the free cumulants  $\kappa_1, \kappa_2$  and the resulting  $(R(z))$  for the three exponents most relevant to SETOL. Higher cumulants follow from the recursion in Eqs. (333)–(334) and need not be written out.

$\alpha = 2$ .

$$C_2 = \frac{\lambda_0 \lambda_{max}}{\lambda_{max} - \lambda_0}, \quad (342)$$

$$\kappa_1 = C_2 \log \frac{\lambda_{max}}{\lambda_0}, \quad (343)$$

$$\kappa_2 = C_2 (\lambda_{max} - \lambda_0) - \kappa_1^2, \quad (344)$$

$$R_{(2)}^{\text{tr}}(z) = \kappa_1 + \kappa_2 z + \mathcal{O}(z^2). \quad (345)$$

$\alpha = 3$ .

$$C_3 = \frac{2 \lambda_0^2 \lambda_{max}^2}{\lambda_{max}^2 - \lambda_0^2}, \quad (346)$$

$$\kappa_1 = \frac{2 \lambda_{max} \lambda_0}{\lambda_{max} + \lambda_0}, \quad (347)$$

$$\kappa_2 = C_3 \log \frac{\lambda_{max}}{\lambda_0} - \kappa_1^2, \quad (348)$$

$$R_{(3)}^{\text{tr}}(z) = \kappa_1 + \kappa_2 z + \mathcal{O}(z^2). \quad (349)$$

$\alpha = 4$ .

$$C_4 = \frac{3 \lambda_0^3 \lambda_{max}^3}{\lambda_{max}^3 - \lambda_0^3}, \quad (350)$$

$$\kappa_1 = \frac{3 \lambda_{max} \lambda_0 (\lambda_{max}^2 - \lambda_0^2)}{2 (\lambda_{max}^3 - \lambda_0^3)}, \quad (351)$$

$$\kappa_2 = C_4 \left( \frac{1}{\lambda_0} - \frac{1}{\lambda_{max}} \right) - \kappa_1^2, \quad (352)$$

$$R_{(4)}^{\text{tr}}(z) = \kappa_1 + \kappa_2 z + \mathcal{O}(z^2). \quad (353)$$

**Interpretation.**  $\kappa_1$  fixes the mean scale of the heavy tail;  $\kappa_2$  sets its leading spread. Because both depend only on the empirical cut-offs  $\lambda_0$  and  $\lambda_{max}$ , the two-term truncation already delivers an accurate  $R$ -transform for free-probability manipulations inside the SETOL framework.

## 3738 A.8 The Inverse-MP (IMP) Model

3739 In this section, we rederive the integral  $G(\lambda)[IMP]$  for the Inverse Marchenko-Pastur (IMP)  
 3740 model, focusing on the branch cut starting at  $z = \kappa/2$  and extending to infinity. This branch cut  
 3741 corresponds to the support of the ESD in this region. We will:

- 3742 1. Explain the presence of the branch cut and its implications.
- 3743 2. Show that  $R(z)[IMP]$  becomes complex along this branch cut because the term under the  
 3744 square root becomes negative.
- 3745 3. Perform the integral  $G(\lambda)[IMP]$ , showing all steps.
- 3746 4. Compute the *Real* part  $\Re[G(\lambda)[IMP]]$

### 3747 A.8.1 The Branch Cut in the IMP Model

3748 The R-transform for the IMP model is given by:

$$R(z)[IMP] = \frac{\kappa - \sqrt{\kappa(\kappa - 2z)}}{z}, \quad (354)$$

3749 where  $\kappa > 0$  is a parameter related to the dimensions of the random matrices under consideration.  
 3750 The function  $\sqrt{\kappa(\kappa - 2z)}$  introduces a branch point at  $z = \kappa/2$  because the argument of the square  
 3751 root becomes zero at this point:

$$\kappa - 2z = 0 \quad \Rightarrow \quad z = \frac{\kappa}{2}. \quad (355)$$

3752 For  $z > \kappa/2$ , the argument  $\kappa - 2z$  becomes negative, and thus the square root becomes imaginary.  
 3753 This leads to a branch cut starting at  $z = \kappa/2$  and extending to  $z = \infty$  along the real axis. This  
 3754 branch cut affects the analyticity of  $R(z)[IMP]$ , and it must be carefully considered in the  
 3755 integral  $G(\lambda)[IMP]$ .

### 3756 A.8.2 $R(z)[IMP]$ is Complex Along the Branch Cut

3757 For  $z > \kappa/2$ , we have:

$$\kappa - 2z < 0 \quad \Rightarrow \quad \sqrt{\kappa(\kappa - 2z)} = \sqrt{-\kappa(2z - \kappa)} = i\sqrt{\kappa(2z - \kappa)}. \quad (356)$$

3758 Therefore,  $R(z)[IMP]$  becomes complex:

$$R(z)[IMP] = \frac{\kappa - i\sqrt{\kappa(2z - \kappa)}}{z} = \frac{\kappa}{z} - i\frac{\sqrt{\kappa(2z - \kappa)}}{z}. \quad (357)$$

3759 This expression shows that  $R(z)[IMP]$  has both real and imaginary parts when  $z > \kappa/2$ .

### 3760 A.8.3 Calculation of $G(\lambda)[IMP]$

3761 We aim to compute the integral:

$$G(\lambda)[IMP] := \int_{\lambda_0}^{\lambda} \Re[R(z)[IMP]] dz, \quad (358)$$

3762 where  $\lambda_0 \geq \kappa/2$ .

3763

Where the Real part of  $R(z)[IMP]$  is

$$\operatorname{Re}[R(z)[IMP]] = \frac{\kappa}{z}. \quad (359)$$

3764

The integral of this is

$$\Re[G(\lambda)[IMP]] = \int_{\lambda_0}^{\lambda} \frac{\kappa}{z}, dz = \kappa [\ln z]_{\lambda_0}^{\lambda} = \kappa (\ln \lambda - \ln \lambda_0). \quad (360)$$

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