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Anonymous authors
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ABSTRACT

Two pressing topics in the theory of deep learning are the interpretation of feature learning mechanisms and the determination of implicit bias of networks in the rich regime. Current theories of rich feature learning effects revolve around networks with one or two trainable layers or deep linear networks. Furthermore, even under such limiting settings, predictions often appear in the form of high-dimensional non-linear equations, which require computationally intensive numerical solutions. Given the many details that go into defining a deep learning problem, this analytical complexity is a significant and often unavoidable challenge. Here, we propose a powerful heuristic route for predicting the data and width scales at which various patterns of feature learning emerge. This form of scale analysis is considerably simpler than such exact theories and reproduces the scaling exponents of various known results. In addition, we make novel predictions on complex toy architectures, such as three-layer non-linear networks and attention heads, thus extending the scope of first-principle theories of deep learning.

1 INTRODUCTION

There is a clear need for a better theoretical understanding of deep learning. However, efforts to construct such theories inevitably suffer from a “curse of details”. Indeed, since any choice of architecture, activation, data measure, and training protocol affects performance, finding a theory with true predictive power that accurately accounts for all those details is unlikely. One workaround is to focus on analytically tractable toy models, an approach that can often uncover interesting fundamental aspects. However, analytical tractability is a fragile, fine-tuned property; thus, a large explainability gap remains between such toy models and more complex data/architecture settings.

An alternative approach focuses on scaling properties of neural networks, which appear more robust. Two well-established examples are empirically predicting network performance by extrapolating learning curves using power laws Kaplan et al. (2020); Hestness et al. (2017), and providing theory-inspired suggestions for hyperparameter transfer techniques Yang et al. (2022); Bordelon et al. (2023). Indeed, it is often the case Cardy (1996) that predicting scaling exponents is easier than predicting exact or approximate behaviors. As a simple toy model of this, consider the integral $\int_{-\infty}^{\infty} dx g(x/P)$. While $g(\cdot)$ needs to be fine-tuned for exact computations, a change of variable reveals a robust linear scaling with P for any $g(\cdot)$.

This work focuses on scaling properties of feature learning. Feature learning, or, more generally, interpretability, have been studied extensively both from the practical and theoretical side. On the practical side, mechanistic interpretability Bereska and Gavves (2024) has provided us with statistical explanations for why some predictions are made and the underlying decision mechanisms. On the theory side, kernel-based ap-

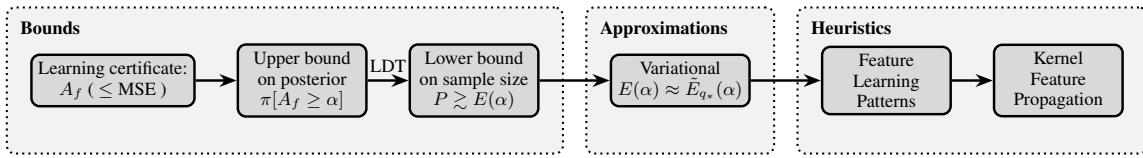


Figure 1: Logical flow of sample complexity derivation. **Bounds:** (i)-(iii) deriving lower bounds on sample complexity using LDT (Sec. 3). **Approximations:** (iv) approximating the intractable lower bound (Sec. 4), **Heuristics:** (v)-(vi) providing heuristic methods for manually computing the approximated bound (Sec. 5). Each section is composed of intermediate steps as detailed in the diagram.

proaches Aitchison (2019); Li and Sompolinsky (2021); Aitchison (2021); Seroussi et al. (2023a); Ariosto et al. (2022); Bordelon and Pehlevan (2022); Rubin et al. (2024; 2025); Ringel et al. (2025) and Saad and Solla type approaches Saad and Solla (1995); Arnaboldi et al. (2023); Bietti et al. (2022) (and their Bayesian counterparts Cui (2025)) allow us to solve simple non-linear teacher-student networks in the rich regime. However, our ability to capture more elaborate and compositional feature learning effects, such as those involving depth and emergence, is hampered by said analytical difficulties.

In this work, we introduce a novel framework addressing the challenging task of making first-principles predictions on sample complexity and feature learning effects in networks trained to equilibrium. The undeniable success of various deep learning models across diverse domains underscores the importance of theoretically predicting the conditions under which these models exhibit failure modes. Accordingly, a main focus of this work is lower-bounding sample complexity. Specifically, we aim to determine the scaling behavior of P_* , the threshold sample size at which learning becomes possible, as a function of input dimension, layer width, regularization, and parametrization choices (e.g., mean-field versus standard scaling).

Our Bayesian approach, capturing networks fully trained using SGLD ¹ Mandt et al. (2017), is described schematically in Fig. 1. It consists of the following steps: (i) we lower bound the test MSE by $(1 - A_f)^2$, where A_f is the alignment of output and target; (ii) we establish an upper bound on the probability to observe good learning (ie, strong alignment $A_f \geq \alpha \approx 1$) in the posterior using the negative-log-probability of the rare event of good learning in the prior; (iii) we leverage an *upper* bound on the prior to obtain a *lower* bound $E(\alpha)$ on the minimal sample size necessary for alignment of at least α ; (iv) we derive a variational approximation, $\tilde{E}_q(\alpha)$, for $E(\alpha)$ with an explicit formula using kernel-adaptation type approximations; (v) we propose *feature learning patterns* as heuristic variational probabilities q and choose such q that minimizes $\tilde{E}_q(\alpha)$; finally (vi) our fully analytic computation of $\tilde{E}_q(\alpha)$ further relies on heuristic scaling relations for how a feature amplified in one layer *propagates* to downstream layers.

Using the above, we re-derive, in a relatively straightforward manner, known results on two-layer networks: sample complexity benefits of rich learning and Grokking transitions. We demonstrate the power of this approach by expanding the scope of tractable models. Specifically, we study non-linear 3-layer networks in the rich regime and predict sample complexity, layer-wise location of learning, and scaling of the number of specializing neurons.

2 SETUP

We consider here several types of feedforward networks, but, for the sake of clarity, we illustrate the main derivation on deep fully connected networks (FCNs) and, later, when we analyze specific problems, augment

¹which can be thought of as a proxy for SGD Mingard et al. (2020)

094 it for convolutional neural networks (CNNs) as needed. Our FCNs are defined by
 095

$$096 \quad f(x) = \sum_{i=1}^{N_{L-1}} w_i^L \sigma(h_i^{L-1}(x)), \quad \text{where } h_i^{l>1}(x) = \sum_{j=1}^{N_{l-1}} W_{ij}^l \sigma(h_j^{l-1}(x)), \quad h_j^1(x) = \sum_{k=1}^d W_{jk}^1 x_k, \quad (1)$$

099 where σ can be any activation function, and we refer to h_i^l 's as *pre-activations*. We consider Bayesian
 100 neural networks, as Bayesian descriptions are a commonly used proxy for network behavior after long-time
 101 stochastic training Wilson and Izmailov (2020); Wilson (2020); Naveh et al. (2021). Alternatively, they
 102 represent an exact solution to Langevin dynamics with weight decay Welling and Teh (2011b). We denote
 103 the target function by y and the training sample size by P , and assume training with Mean Squared Error
 104 (MSE) loss. The quadratic weight decay for each layer l is set to $\kappa N_{l-1}/\sigma_l^2$, where κ is the ridge parameter
 105 and $N_0 = d$ is the input dimension. This choice of weight decay results in a Gaussian prior distribution for
 106 the weights given by $W_{i,j}^l \sim \mathcal{N}(0, \sigma_l^2/N_{l-1})$ for $i = 1, \dots, N_l$, $j = 1, \dots, N_{l-1}$. The possible outputs f of
 107 such a network, given y and P , are then distributed according to the posterior:

$$108 \quad \pi(f | y, P) = \frac{1}{Z} \exp \left(-\frac{1}{2\kappa} \sum_{\nu=1}^P [f(x_\nu) - y(x_\nu)]^2 \right) p_0(f), \quad (2)$$

111 where Z is the normalization constant, $\{x_\nu\}_{\nu=1}^P$ is the training dataset of size P , and $p_0(f)$ is the prior
 112 defined as $p_0(f) = \int d\Theta p(\Theta) \delta[f - f_\Theta]$, determined by the weight decay. Here, Θ is the collection of
 113 all network weights, and $p(\Theta)$ corresponds to the density of the prior weight distribution, which we take
 114 to be Gaussian with a diagonal covariance, representing quadratic weight decay, and f_Θ is the network
 115 architecture with weights Θ . We further set $p(\Theta)$ such that pre-activations are all $\mathcal{O}(1)$ under the prior He
 116 et al. (2015). For classification tasks see App. A.2. As a measure for learning, we consider an observable,
 117 which we refer to as *alignment*, given by

$$118 \quad A_f := \langle f, y \rangle / \langle y, y \rangle, \quad (3)$$

119 where $\langle g, h \rangle = \int d\mu_x g(x)h(x)$ is the functional inner product, and $d\mu_x$ is some test measure, which, con-
 120 veniently, does not need to be the measure from which the training set was drawn. We similarly define
 121 $\langle g, K, h \rangle = \int d\mu_x d\mu_{x'} g(x)K(x, x')h(x')$ for any kernel K . Alignment represents the extent to which the
 122 network learns a function that is proportional to the target. It bounds the test MSE via the Cauchy–Schwarz
 123 inequality $\int d\mu_x (f(x) - y(x))^2 \geq \langle y, y \rangle (A_f - 1)^2$. Having $A_f \approx 1$ is thus a necessary condition for
 124 successful learning.

125 3 ALIGNMENT AND SAMPLE COMPLEXITY

126 We turn to analyze sample complexity via an upper bound on the probability of finding $A_f \geq \alpha$ for $\alpha \approx 1$.
 127 We begin with a theoretical bound on the posterior that mainly depends on the chance that a random network,
 128 chosen from the prior, produces an alignment of at least α . We denote the prior and posterior alignment
 129 probabilities by $\Pr_{p_0}[A_f \geq \alpha]$ and $\Pr_\pi[A_f \geq \alpha]$ respectively. Following simple arguments (see App. A
 130 and App. A.2 for generalization to classification.), we obtain the following bound on the log posterior²

$$131 \quad \log(\Pr_\pi[A_f \geq \alpha]) < Pk / (2\kappa) + \log(\Pr_{p_0}[A_f \geq \alpha]), \quad (4)$$

132 where $k = P^{-1} \sum_{\nu=1}^P \mathbb{E}_{p_0}[(f(x_\nu) - y(x_\nu))^2]$ is the only training-set dependent quantity and is generally
 133 of order one. The Bayesian interpretation of successful learning is having $\Pr_\pi[A_f \geq \alpha] \approx \mathcal{O}(1)$. Since
 134 a random network is unlikely to achieve strong alignment, $\log \Pr_{p_0}[A_f \geq \alpha]$ would typically be highly
 135 negative for large α . Therefore, a sufficiently large data term is required to cancel this effect. Explicitly,

$$136 \quad P \gtrsim -2\kappa \log \Pr_{p_0}[A_f \geq \alpha] / k. \quad (5)$$

137
 138 ²See also Lavie and Ringel (2025), for a similar data-agnostic bound in the context of lazy learning.

141 Thus, up to the ridge parameter and the $\mathcal{O}(1)$ factor k , depending on the training set, the log probability
 142 of prior alignment with the target lower bounds the sample complexity. Here, it is worth noting that the
 143 bound becomes tight when overfitting effects are small, which is typically the case for $k/\kappa \sim \mathcal{O}(1)$. Taking
 144 $\kappa \rightarrow 0$ encourages overfitting (though often benignly Bartlett et al. (2020)) and trivializes this bound. We
 145 conjecture that, in this case, κ should be kept $\mathcal{O}(1)$ based on the effective ridge treatment Canatar et al.
 146 (2021); Cohen et al. (2021); Bartlett et al. (2020). Establishing this conjecture is outside the scope of this
 147 work. From a PAC-Bayesian perspective, an analogous bound would require P to be much larger than the
 148 KL-divergence between the prior and posterior (e.g. McAllester (1999)).³. More recently, prior-posterior
 149 relations have been studied in the context of complex Boolean functions Mingard et al. (2025).

150 Following the Chernoff inequality, we can find an upper bound for the probability (and a lower bound for
 151 P) via

$$152 \quad P \geq -2\kappa/k \log \Pr_{p_0} [A_f \geq \alpha] \geq 2\kappa/k E(\alpha), \quad E(\alpha) = -\log \inf_{t>0} e^{-t\alpha} \mathbb{E}_{p_0} [e^{tA_f}]. \quad (6)$$

154 Where we refer to $E(\alpha)$ as the *energy*. We can thus express the minimal sample size necessary for learning
 155, P_* , through the energy as $P_* \propto E(\alpha)$. In App. B, we provide an asymptotically exact solution for
 156 $E(\alpha)$, and compute it explicitly for a two layer network. We also argue and demonstrate that our bound is
 157 inherently tied to feature learning. Indeed, a network sampled from the prior that achieves such alignment
 158 is a statistical outlier, driven by the emergence of an internal structure which mimics feature learning (see
 159 also Fig. 2). Nevertheless, such a direct LDT approach is computationally prohibitive in most cases of interest.
 160 We therefore introduce a heuristic LDT-based method for evaluating P_* . This method not only enables
 161 predicting the scaling of P_* but also the feature learning effects that lead to successful learning.

162 In this section, we adopt a variational approach to estimating P_* by comparing different modes of feature
 163 learning⁴ under a certain loss (see (9) below). While many approaches predict different feature learning
 164 mechanisms Pacelli et al. (2023); Fischer et al. (2024); Meegen and Sompolinsky (2024); Buzaglo et al.
 165 (2025); Li and Sompolinsky (2021); Seroussi et al. (2023b); Rubin et al. (2025; 2024), they are often case-
 166 dependent, highly detailed, and complex. Thus, we propose a method that abstracts key feature learning
 167 mechanisms from these frameworks into distinct, comparable patterns.

168 4 VARIATIONAL ANALYSIS

171 Our next objective is to make the sample complexity bound tractable. This requires estimating the prior
 172 probability term, $\Pr_{p_0} [A_f \geq \alpha]$, for alignments $\alpha \approx 1$. As a first step, we simplify this by relating the
 173 cumulative distribution function to the probability density denoted by $p_{A_f}(\alpha)$. As shown in App. A.3, for
 174 large alignments, we have $E(\alpha) \approx -\log p_{A_f}(\alpha)$. This allows us to re-express P_* in terms of the density:
 175 $P_* = -2\kappa \log p_{A_f}(\alpha)/k$. However, computing $p_{A_f}(\alpha)$ directly remains intractable. We therefore turn to
 176 a variational approach to estimate it. As explained in the next section, we wish to express the variational
 177 probability density in terms of pre-activations h (1). Accordingly, in App. C.1, we follow standard statistical
 178 mechanics techniques to express this density as

$$179 \quad p_{A_f}(\alpha) = \int Dh \exp[-H_{p,\alpha}(h)]/Z_p, \quad \text{where} \quad Z_p = \int_{-\infty}^{\infty} d\alpha \int Dh \exp[-H_{p,\alpha}(h)]. \quad (7)$$

182 We comment that the above equation explicitly constitutes a definition of $H_{p,\alpha}$, namely, for every α one
 183 can find a function $H_{p,\alpha}(h)$ and normalizing constant Z_p such that (7) holds. Further requiring that

184 ³Following the data-processing-inequality, one can lower-bound the KL-divergence between the full prior and poste-
 185 rior probabilities by the KL-divergence of a coarser probability of an $A_f \geq \alpha$ event in the prior and posterior. The latter
 186 KL divergence is given by $-\log \Pr_{p_0} [A_f \geq \alpha]$

187 ⁴Viewed here formally as emergent weight/pre-activation structures enabling the outlier.

188 $\min_h H_{p,\alpha}(h) = 0$ ensures the uniqueness of this definition. Similarly, the above implies a measure over
 189 h 's given by $\exp[-H_{p,\alpha}(h)]/\int \mathcal{D}h \exp[-H_{p,\alpha}(h)]$. We next approximate this measure per α by an
 190 analytically tractable variational estimate, q . Here too we follow the same notation as in (7), so that for any
 191 q, α we define $q_\alpha(h) := e^{-H_{q,\alpha}(h)}/Z_{q,\alpha} = \int \mathcal{D}h e^{-H_{q,\alpha}(h)}$. The variational computation
 192 follows by looking for $q_\alpha(h)$ which minimizes the KL divergence between the measure on h which defines
 193 p_{A_f} , and q . The KL divergence can also be used in the estimation of $E(\alpha) := -\log(p_{A_f}(\alpha))$, following
 194 the Feynman–Bogoliubov inequality Kuzemsky (2015); Bogolubov and Jr (2009); Huber (1968). Here we
 195 provide a brief description – for the full derivation see App. C.2. By applying the Feynman–Bogoliubov
 196 inequality, we obtain an upper bound on $E(\alpha)$

$$197 \quad E(\alpha) \approx \min_{q_\alpha} (\log(Z_p/Z_{q,\alpha}) + \tilde{E}_q(\alpha)), \quad \tilde{E}_q(\alpha) = \mathbb{E}_{h \sim q_\alpha} [H_{p,\alpha}(h) - H_{q,\alpha}(h)] \quad (8)$$

199 We argue in App. C.4 that for $\alpha \approx 1$, the log terms are subleading w.r.t. $\tilde{E}_q(\alpha)$. Defining $q_{*,\alpha}$ to be the
 200 measure that minimizes $\tilde{E}_q(\alpha)$, we obtain $E(\alpha) \approx \tilde{E}_{q_*}(\alpha)$.

202 Next, we turn to estimating the variational energy $\tilde{E}_q(\alpha)$ Eq. (8) for $\alpha \sim 1$, omitting all α indices for brevity.
 203 In App. C.1 we simplify p_{A_f} , and show that the distribution in each layer depends only on the previous
 204 through a fluctuating non-linear operator. Next, we assume that this kernel is weakly fluctuating, and replace
 205 it with its expectation w.r.t. the variational distribution. This choice approximation aligns with various
 206 works on deep non-linear networks, where layer-wise kernels are identified as the relevant and sufficient set
 207 of order parameters Rubin et al. (2025); Fischer et al. (2024); Seroussi et al. (2023b); Ringel et al. (2025).
 208 We further take a decoupled Gaussian variational ansatz so that $q(h) = \prod_{l=1}^{L-1} \prod_{i=1}^{N_l} q_{l,i}(h_i^l)$ where $q_{l,i}$ is
 209 Gaussian with mean $\mu_{l,i}$ and variance $Q_{l,i}$. As shown in App. C.3, the variational energy estimate is then
 210 given by

$$211 \quad \tilde{E}_q \propto \sum_{l=1}^{L-1} \sum_{i=1}^{N_l} \underbrace{\left(\mathbb{E}_{h \sim \mathcal{N}(\mu_{l,i}, Q_{l,i})} [\langle h, K_{l-1}^{-1} - Q_{l,i}^{-1}, h \rangle] + \langle \mu_{l,i}, Q_{l,i}^{-1}, \mu_{l,i} \rangle \right)}_{=: \Delta_{l,i}} + \underbrace{\langle y, K_{L-1}, y \rangle^{-1}}_{=: a_y}, \quad (9)$$

215 where we define

$$217 \quad K_{l>0}(x, x') = \frac{\sigma_{l+1}^2}{N_l} \sum_{i=1}^{N_l} \mathbb{E}_{h_i^l \sim q_{l,i}} [\sigma(h_i^l(x)) \sigma(h_i^l(x'))], \quad K_0(x, x') = \frac{\sigma_1^2}{d} x \cdot x'. \quad (10)$$

220 Here, the $\Delta_{l,i}$ terms arise from the difference between the approximated kernel and the actual one, and the
 221 a_y term results from enforcing an alignment $\alpha \approx 1$. Requiring that q minimize \tilde{E}_q and $\alpha \approx 1$, we estimate
 222 $\tilde{E}_q \propto E(\alpha \approx 1) \propto P_*$. Another interpretation of $\Delta_{l,i}$, discussed in App. D, is the excess weight due to
 223 feature learning. This viewpoint is useful for feature learning patterns involving circuits, as the latter have a
 224 sharp imprint in weight-space. The above kernel viewpoint is, however, more general and can be used both
 225 for circuits and for more distributed learning patterns.

227 5 HEURISTICS FOR MANUAL COMPUTATION OF VARIATIONAL APPROXIMATION

229 5.1 FEATURE LEARNING PATTERNS

231 While the above variational approach allows a variety of candidate q 's, we focus on the previously mentioned
 232 set of feature-learning scenarios that have been extensively studied in the literature. Although this subset
 233 may appear restrictive, by varying behaviors among layers and between different neurons of the same layer,
 234 it already captures a wide range of phenomena. We then need to compare the variational energy (\tilde{E}_q), as

235 detailed in Sec. 4, for such combinations and select the minimizer. The optimal pattern is an indication
 236 of the feature learning that emerges in the network to enable strong alignment, as motivated in App. A.3.
 237 Concretely, per layer and neuron pre-activation ($h_i^l(x)$), we allow one of the following choices, as illustrated
 238 in Fig.
 239

240 **(1) Gaussian Process (GP).** Here, $q_{l,i}$ is a Gaussian process (GP) so that $h_{l,i} \sim \mathcal{N}(0, K_{l-1})$ with K_{l-1}
 241 defined in (10). This choice defines the “base model” of feature learning. For FCNs,⁵ it implies that the
 242 network propagates feature structure forward without altering latent features (see Sec. 5.2). When all layers
 243 and neurons follow this distribution, the network reduces to the neural network GP (NNGP) Neal (1996),
 244 where no feature learning occurs. Introducing any of the patterns below in a subset of neurons enables
 245 feature learning to emerge.
 246

247 **(2) Gaussian Feature Learning (GFL).** In this scenario, pre-activations remain Gaussian with zero mean,
 248 but the covariance is modified relative to the GP scenario (1): the kernel of the previous layer is amplified
 249 by a factor D in the direction of a specific feature (e.g. an eigenfunction of K_{l-1}) Φ_*^l .⁶ Thus, here too, the
 250 distribution is a GP but with a different covariance $Q_{l,i}$ given by
 251

$$Q_{l,i}(x, x') = K_{l-1}(x, x') + D \langle \Phi_*^l, K_{l-1}, \Phi_*^l \rangle \Phi_*^l(x) \Phi_*^l(x'). \quad (11)$$

252 **(3) Specialization.** In this scenario, a given neuron specializes to a particular feature Φ_*^l with proportionality
 253 constant $\mu_{l,i}$. This pattern corresponds to a Gaussian distribution which is sharply peaked around a
 254 non-zero mean $\mu_{l,i} \Phi_*^l$.⁷ Explicitly, we define the distribution of the specialized neuron as
 255

$$q_{l,i}(\langle h_i^l, \Phi_*^l \rangle) = \delta[\langle h_i^l, \Phi_*^l \rangle - \mu_{l,i}], \quad q_{l,i}(\langle h_i^l, \Phi_\perp^l \rangle) = \mathcal{N}(0, \langle \phi_\perp^l, K_{l-1}, \Phi_\perp^l \rangle). \quad (12)$$

258 5.2 LAYER-WISE FEATURE PROPAGATION

260 Since the variational energy of each layer depends on the kernel of the previous layer, an important element
 261 in our heuristic is understanding how the choice of pattern in a given layer affects the kernel and its spectrum
 262 in the subsequent layer. To this end, we define feature learning as any deviation from the baseline GP pattern
 263 (see Sec. 5.1), such as introducing a non-zero mean to the distribution (i.e., specialization) or altering its
 264 covariance structure (i.e., GFL). In our framework, a “feature” refers either to the mean $\mu_{l,i}$ of $q_{l,i}$ or to an
 265 eigenfunction of its covariance operator $Q_{l,i}(x, x')$.
 266

267 We now outline several key claims concerning how features typically propagate between layers in FCNs. In
 268 this context, we consider a data measure that is i.i.d. Gaussian with zero mean and variance 1, not because
 269 it approximates the data well, but rather because it provides an unbiased baseline (see also Lavie and Ringel
 270 (2025)) for measuring function overlaps. Depending on the input, other choices can also be considered
 271 (e.g. permutation-symmetric measures over discrete tokens Lavie et al. (2024)). The following claims with
 272 their justifications should be understood as heuristic principles or rationalizations of empirically observed
 273 phenomena. Proving them in general or augmenting for different architectures is left for future work. For
 274 further details and empirical results, see App. C.5.
 275

276 **Claim (i): Neuron specialization creates a spectral spike.** Assume that M neurons in layer l specialize
 277 on a single feature $\Phi_*^l(x)$, the subsequent kernel K_l develops a new, dominant spectral feature
 278 corresponding to $\sigma(\Phi_*^l(x))$. The corresponding RKHS norm of this feature is amplified, scaling
 279

⁵For CNNs, even in the lazy regime, deeper kernels have different input scope and hence do generate new structure.

⁶One may also consider generalizations to several features.

⁷Taking equilibrated networks and increasing the amount of data, specialization was shown in Rubin et al. (2024) to emerge as a first-order phase transition where the average of preactivations suddenly shifts to $\mu_{l,i}$. This behavior was further associated with Grokking, suggesting a potential specialization-grokking link.

282 as $\mathcal{O}(N_l/M)$. **Justification:** When M neurons specialize, the next layer's kernel is approximately
 283 $K_l(x, x') = A(x, x') + \frac{M}{N_l} \sigma(\Phi_*^l(x)) \sigma(\Phi_*^l(x'))$, where A is the contribution from the non-specialized neurons.
 284 Treating the specialization term as a rank-1 update, the Sherman-Morrison formula shows that its
 285 RKHS norm becomes $(R_A^{-1} + M/N)^{-1}$, where R_A is the RKHS norm of A , which satisfies $R_A^{-1} \ll M/N$
 286 in typical high-dimensional settings.
 287

288 **Claim (ii): Amplified features in the pre-activation kernel create amplified higher-order features in
 289 the post-activation kernel.** If a feature $\Phi_*^l(x)$ in kernel K_l has its eigenvalue enhanced by a factor D (i.e.,
 290 $\lambda_* \rightarrow \lambda_* D$), then the corresponding m -th order power of this feature $(\Phi_*^l)^m(x)$ will have the bulk of its
 291 spectral decomposition, under the downstream kernel, shifted up by D^m , with similar effect on the inverse
 292 RKHS norm. **Justification:** A Taylor expansion of K_{l+1} in terms of the eigenfunctions of K_l shows that
 293 the term corresponding to $(\Phi_*^l)^m(x)$ will have a coefficient scaling with $(\lambda_* D)^m$. We argue that this term is
 294 difficult to span using other terms in this expansion, allowing us to treat it as a spectral spike and analyze it
 295 similarly to Claim (i). A numerical demonstration of this effect is shown in Fig. 5.
 296

297 **Claim (iii): Lazy layers preserve the relative scale of features from the previous layer.** In the absence
 298 of feature learning, a properly normalized lazy layer approximately preserves the eigenspectrum of the
 299 previous kernel. If a feature $\Phi_*^l(x)$ has an eigenvalue λ_* with respect to the pre-activation kernel given by
 300 K_{l-1} , its effective eigenvalue with respect to the post-activation kernel K_l will also be proportional to λ_* .
 301 **Justification:** Follows from Claim (ii) taking $D = 1$.
 302

303 Propagation rules for FCNs

304 (1) **Specialization:** Layer l specialized M neurons on Φ_*^l . For any feature Φ satisfying $\langle \sigma(\Phi_*^l), \Phi \rangle \neq$
 305 0, we approximate $\langle \Phi, K_l^{-1}, \Phi \rangle \propto \left[\sum_{i \text{ sp.}} \frac{\mu_{i,l}^2}{N_l} \right]^{-1}$, where we sum over all specializing neurons.
 306 (2) **GFL:** Layer l amplified fluctuation along Φ_*^l by D so that $\langle \Phi_*^l, K_l^{-1}, \Phi_*^l \rangle = (D\lambda_*)^{-1}$, where λ_*
 307 is the GP value of the inner product. Then for any m we have $\langle (\Phi_*^l)^m, K_l^{-1}, (\Phi_*^l)^m \rangle \propto (D\lambda_*)^{-m}$.
 308

311 6 CONCRETE EXAMPLES

312 We now apply the heuristic principles of Sec. 4, 5.1, 5.2 to derive sample complexity bounds in a few examples.
 313 In App. E.1, we benchmark our method on two-layer FCNs and simple CNNs with non-overlapping
 314 patches. There we reproduce both the sample complexity exponent $P_* = d^{3/4}$ identified for CNNs in Ringel
 315 et al. (2025) and further predict that $P_* = d$ for two-layer FCNs studying a Hermite-3 target as well as the
 316 scaling of the number of specializing neurons with width (see Fig. 2). The latter is also a setting for which
 317 the prior's upper bound can be computed directly from $E(\alpha)$ using Large Deviation Theory, leading to a
 318 good match with experiment (Fig. 2 panel (a)).
 319

320 Going to what we believe is beyond the current analytical state of the art, in App. E.3, we predict a $P_* = \sqrt{L}$,
 321 where L is the context length, of a softmax attention layer learning a cubic target (see Fig. 3). Another such
 322 instance, discussed in detail below, is that of a 3-layer non-linear network learning a non-linear target. In
 323 App. A.2 we show that this approach can be extended to classification tasks as well. In App. E.2 we apply
 324 our heuristics to a concrete setting, of a two-layer ReLU network trained on a parity task. We find there as
 325 well are able to predict the emergent feature pattern, which qualitatively differs from erf networks. Rather
 326 than identifying the scaling number of specializing neurons, we find that there is a finite number of neurons
 327 and we are able to predict their scale.
 328

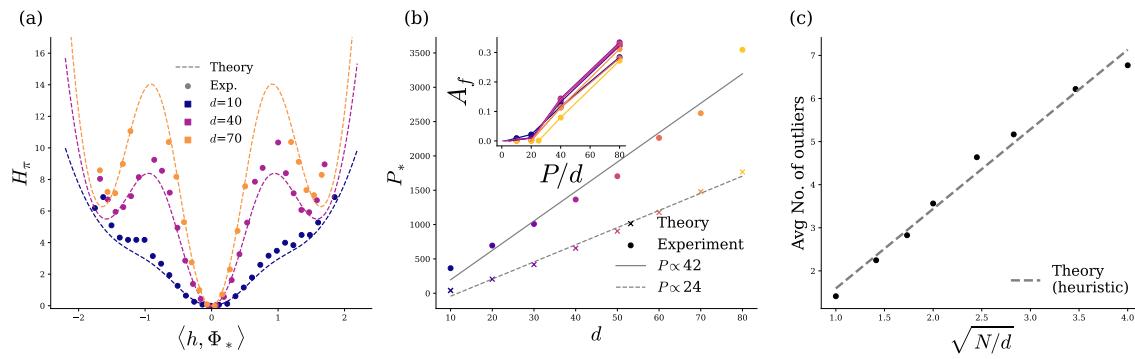


Figure 2: Numerical and experimental results for a two-layer erf network trained on the normalized third Hermite polynomial ($m = 3$). In panel (a) we compare the experimental results and exact theoretical predictions (computed utilizing LDT, see App. B) for the distribution of the alignment of the hidden layer pre-activation with the linear feature. Here we follow the same notation as in (7), so that H_π is the negative log posterior of the preactivations up to an additive constant that enforces zero minimum. We also find the pre-activation distribution corresponds to $q(h)$ for $q \sim \text{M-Sp}$, as predicted by our heuristic approach. Panel (b) compares theoretical and experimental predictions for P_* , defined as alignment $\alpha > 0.1$ (inset shows alignment as a function of sample size). Both theoretical and experimental results agree on $P_* \propto d$. In (c), we increase N and keep P and d fixed, and plot the number of specialized neurons in the hidden layer. In agreement with our heuristic predictions, the number of neurons increases linearly with $\sqrt{N/d}$.

6.1 THE THREE-LAYER NETWORK

Here we consider a three-layer FCNs given by

$$f(x) = \sum_{i=1}^{N_2} a_i \sigma \left(\sum_{j=1}^{N_1} w_{ij}^{(2)} \sigma(w_j^{(1)} \cdot x) \right), \quad (13)$$

where $x \in \mathbb{R}^d$ is drawn from $\mathcal{N}(0, I_d)$. We train these networks on a polynomial target of degree m given by $y(x) = H_m(w_* \cdot x)$ where H_m is the m -th probabilist Hermite polynomial, which is the standard polynomial choice under our choice of data measure, and $w_* \in \mathbb{R}^S$ is some normalized vector. The networks are trained via Langevin dynamics Welling and Teh (2011b), with ridge parameter κ , quadratic weight decay, and standard scaling. For an extension to mean-field scaling, see App. E.1.1.

As a starting point for our analysis, consider the simplest pattern ($q = \text{GP-GP}$), having two GP/lazy layers where taking an l 'th layer to be lazy means $Q_{l,i} = K_{l-1}$ and $\mu_{l,i} = 0$. Following the choice of pattern, our goal is to estimate the scaling of \tilde{E}_q . Examining Eq. (9), we find that the $\Delta_{l=1,2,i}$ contributions all cancel by our above choice of Q 's and μ 's. The only non-zero contribution thus comes from the final layer and is given by the inverse of $\langle y, K_2, y \rangle$. Because of lazy learning, $K_2(x, x')$ is a standard dot product FCN kernel which can be expanded as $\sum_{n=1}^{\infty} a_n (x \cdot x'/d)^n$, with $a_n = O(1)$ w.r.t. $N_{1,2}, d, P$. It can then be shown that $\langle y, K_2, y \rangle = O(d^{-m})$. Leading to $\tilde{E}_{\text{GP-GP}} = a_y \propto d^m$.

Next, we consider a feature learning pattern wherein the first layer is GP distributed but the second has feature learning ($q = \text{GP-Sp}$). Specifically, for the $l = 1$ layer, we take $Q_{1,i} = K_0$; $\mu_{1,i} = 0$ thereby nullifying again $\Delta_{1,0}$ in Eq. 9 for \tilde{E}_q . For the second layer, we assume M_2 specializing neurons (e.g. $i = 1..M_2$) which fluctuate around the linear feature $(w_* \cdot x)$, while others are lazy, namely $Q_{2,i > M_2} =$

376 $K_1, \mu_{2,i>M_2} = 0$ and $Q_{2,i=1..M_2} = K_1, \mu_{2,i=1..M_2}(x) = (w_* \cdot x)$. Examining $\sum_{i=1}^{N_2} \Delta_{2,i}$ in Eq. 9, we
 377 get zero contributions from $\Delta_{2,i>M_2} = 0$ and $M_2 \langle (w_* \cdot x), K_1^{-1}, (w_* \cdot x) \rangle$ from $i = 1..M_2$. As K_1 is
 378 again a simple FCN dot product kernel with no feature learning effects, normalized linear functions such
 379 as $w_* \cdot x$ have an $O(d)$ RKHS norm. We thus obtain an overall contribution to \tilde{E}_q from the $l = 2$ layer
 380 equal to $M_2 d$. Finally, we need to estimate $a_y = \langle y | K_2 | y \rangle^{-1}$. Note that K_2 is not a standard FCN kernel
 381 anymore, since Q_2 , which contains target information, is used in its definition (Eq. 10). According to our
 382 feature propagation rule (i), with $\Phi_* = (w_* \cdot x)$, we have $a_y = N_2/M_2$. Given M_2 , we thus obtain a
 383 variational energy of $M_2 d + N_2/M_2$. We next need to minimize over free parameters, namely M_2 leading
 384 to $M_2 = \sqrt{N_2/d}$ and finally $\tilde{E}_{\text{GP-Sp.}} = \sqrt{N_2 d}$. Provided N_2 scales less than d^{2m-1} ($N_2 = o(d^{2m-1})$),
 385 this pattern is favorable to **GP – GP**.

386 Finally, we consider what turns out to be the favorable pattern consisting of M_1 neurons specializing on
 387 $(w_* \cdot x)$ in the first layer and all neurons in the second layer specializing $H e_m(w_* \cdot x)$ in the second layer,
 388 with a small proportionality constant $\mu_{2,i} = \pm \sqrt{\beta/N_2}$ ($q = \text{Sp.-Mag.}$). We refer to the second-layer pattern
 389 as magnetization. Following straightforward adaptation previous argument to this pattern, the variational
 390 energy for this pattern as well as others, for $m = 3$, can be found in Table 1.
 391

Feature Pattern	Δ_1	Δ_2	a_y	Minimizing Parameters	\tilde{E}
GP-GP	0	0	d^3	–	d^3
GP-Sp.	0	$M_2 d$	$\frac{N_2}{M_2}$	$M_2 = \sqrt{\frac{N_2}{d}}$	$\sqrt{N_2 d}$
Sp.-Mag.	$M_1 d$	$\frac{N_1}{M_1} \beta$	$\frac{N_2}{\beta}$	$\beta = \left(\frac{N_2^2}{N_1 d} \right)^{1/3}, \quad M_1 = \left(\frac{N_2 N_1}{d^2} \right)^{1/3}$	$(N_1 N_2 d)^{1/3}$

400 Table 1: Variational energy \tilde{E} for different choices of feature-learning patterns in a three-layer FCN trained
 401 on $y(x) = \text{He}_3(w_* \cdot x)$. The patterns shown here are (first/second layer): GP-GP, GP-Specialization, and
 402 Specialization-Magnetization. For each pattern, the components of the variational energy (Δ_1, Δ_2, a_y)
 403 together with the corresponding minimizing parameters are shown. We comment that the GP-GP pattern is
 404 favorable only for $d > N_2^5$, and otherwise feature learning will emerge.
 405

406 In the non-GP q patterns, we obtain the same scaling of \tilde{E}_q in the proportional limit ($N_1 \propto N_2 \propto d$),
 407 namely, $P_*/\kappa \propto d$. This observation is validated experimentally in Fig. 3, where the transition to non-zero
 408 alignment becomes sharper in the thermodynamic limit ($d \rightarrow \infty$). However, the mechanism by which this
 409 scaling is realized changes. In the specialization-magnetization pattern the sample complexity scales with
 410 $N_1^{1/3}$, therefore, it increases with N_1 . However, under the GP-specialization pattern, sample complexity
 411 does not scale with N_1 , making this pattern preferable. This prediction is in line with experimental results
 412 (see Figs. 8 and 3 panel (c)) where increasing N_1 causes the described change in feature learning patterns.
 413 Our prediction also accurately determines the scaling of the number of specializing neurons with N_1 .

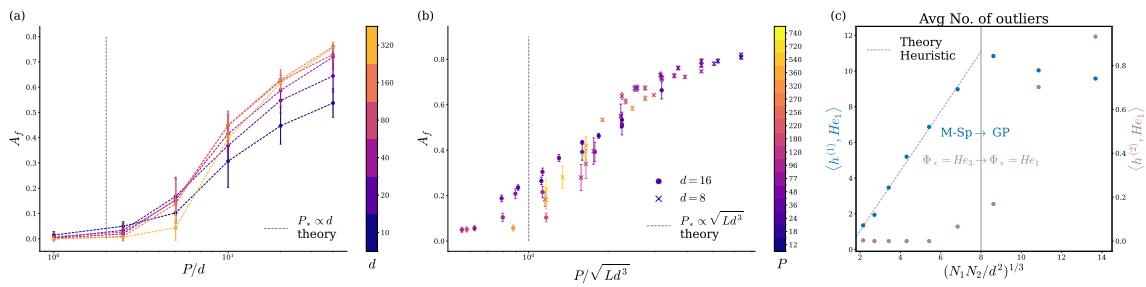
414 6.2 SOFTMAX ATTENTION

415 Here, we consider an attention block of the form

$$416 \quad f(X) = \frac{1}{\sqrt{L}} \sum_{h=1}^H \sum_{a,b=1}^L @_{ab;h}(X) (w_h \cdot x^b) \quad @_{ab;h}(X) = e^{[x^a]^\top A_h x^b} \left(\sum_{c=1}^L e^{[x^a]^\top A_h x^c} \right)^{-1}, \quad (14)$$

417 where $X \in \mathbb{R}^{L \times d}$, $A \in \mathbb{R}^{d \times d}$, and $x^a \in \mathbb{R}^d$ is the a -th row of X , and $w_h \in \mathbb{R}^d$. Our prior on network
 418 weights is $\prod_{h=1}^H \mathcal{N}(0, I_{d^2}/d^2; A_h) \mathcal{N}(0, I_d/(dH); w_h)$. The only dependence on the context length L arises

423 from the pre-factor $1/\sqrt{L}$, which ensures that for $X_i^a \sim \mathcal{N}(0, 1)$, we have $f(X) = \mathcal{O}(1)$. The target
 424 function is given by $y(X) = \sum_{a,b} \frac{1}{\sqrt{L(L-1)}} x_1^a x_2^b x_3^b$, also normalized to be $\mathcal{O}(1)$. Following our approach,
 425 we propose two patterns for this architecture: GP (or lazy learning) and specialization (where we take
 426 $A_h \sim \mathcal{N}(\mu \sigma_x \otimes I_{(d-2)}, I_{d^2})$ for $\sigma_x = [1, 0; 0, 1]$ and optimize over μ). As detailed in E.3, the variational
 427 energy scales as Ld^3 for the GP pattern and as $\sqrt{H}Ld^3$ for the specialization pattern, the latter thus being
 428 favorable for H scaling less than $\sqrt{Ld^3}$. As shown in Fig. 3, this scaling of P with L and d indeed matches
 429 the dependence of the sample complexity on L .
 430



441 **Figure 3: Sample complexity:** Heuristic predictions accurately capture sample complexity in both three-
 442 layer erf FCNs and softmax attention heads, as well as feature learning scaling. Panels (a),(b) both track
 443 how the network alignment changes as a function of the ratio between the sample size, P , and the predicted
 444 sample complexity- P/d for the FCN in panel (a), and $P/\sqrt{Ld^3}$ for the attention head in panel (b). In
 445 both cases, we observe that the alignment collapses onto a single curve, confirming the predicted sample
 446 complexity, where good alignment is achieved. See Fig. 9 for comparison to MSE. See E.3 and F.1
 447 for experimental details. **Feature learning patterns:** Panel (c) tracks the number of linearly specialized
 448 neurons, in both the first (blue) and second (purple) layers as the first-layer width N_1 varies (with fixed P, d
 449 and N_2). The number of first-layer specializing neurons initially follows the predicted $(N_1/d)^{(1/3)}$ scaling
 450 before the predicted transition occurs, where second-layer neurons begin to specialize on the linear feature
 451 rather than the cubic one, and the first layer neurons approach the GP distribution.
 452

453 7 DISCUSSION

454 This paper presents a novel methodology for analyzing the scaling behavior of sample complexity, through
 455 which we can also understand how distinct learning mechanisms emerge. Its strength lies in abstracting
 456 away from fine-grained details to isolate the core principles at play. By providing a common language for
 457 disparate phenomena, our work aims to unify fragmented theoretical perspectives, paving the way for an
 458 accessible and cohesive theory of representation learning. We hope such a strategy would remove barriers
 459 and expedite connections between mechanistic interpretability and first-principles scientific approaches.
 460

461 **Limitations.** Notwithstanding our contributions, several avenues for improvement remain. In particular,
 462 extending the approach to overfitting patterns, quantifying feature propagation in more general CNNs and
 463 transformers, and addressing multi-feature interaction effects as those appearing in the context of superpo-
 464 sition Elhage et al. (2022). It would also be desirable to extend our heuristic to dynamics of learning, po-
 465 tentially drawing insights from previous work relating equilibrium and dynamical phenomena Power et al.
 466 (2022); Rubin et al. (2024); Bahri et al. (2024); Nam et al. (2024). Since Bayesian convergence times can
 467 be exceptionally slow, correctly predicting the emergence of feature learning in early stages of training may
 468 also be highly advantageous. Finally, in some cases, such as under mean-field scaling, overfitting effects can
 469 emerge. It would therefore be valuable to extend our approach to account for patterns that lead to overfitting.

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