Phase Transitions for Feature Learning in Neural Networks

Zihao Wang (Stanford University)

Center for Computational Mathematics, Flatiron Institute
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Joint work with Andrea Montanari
(Stanford University)

Empirical success

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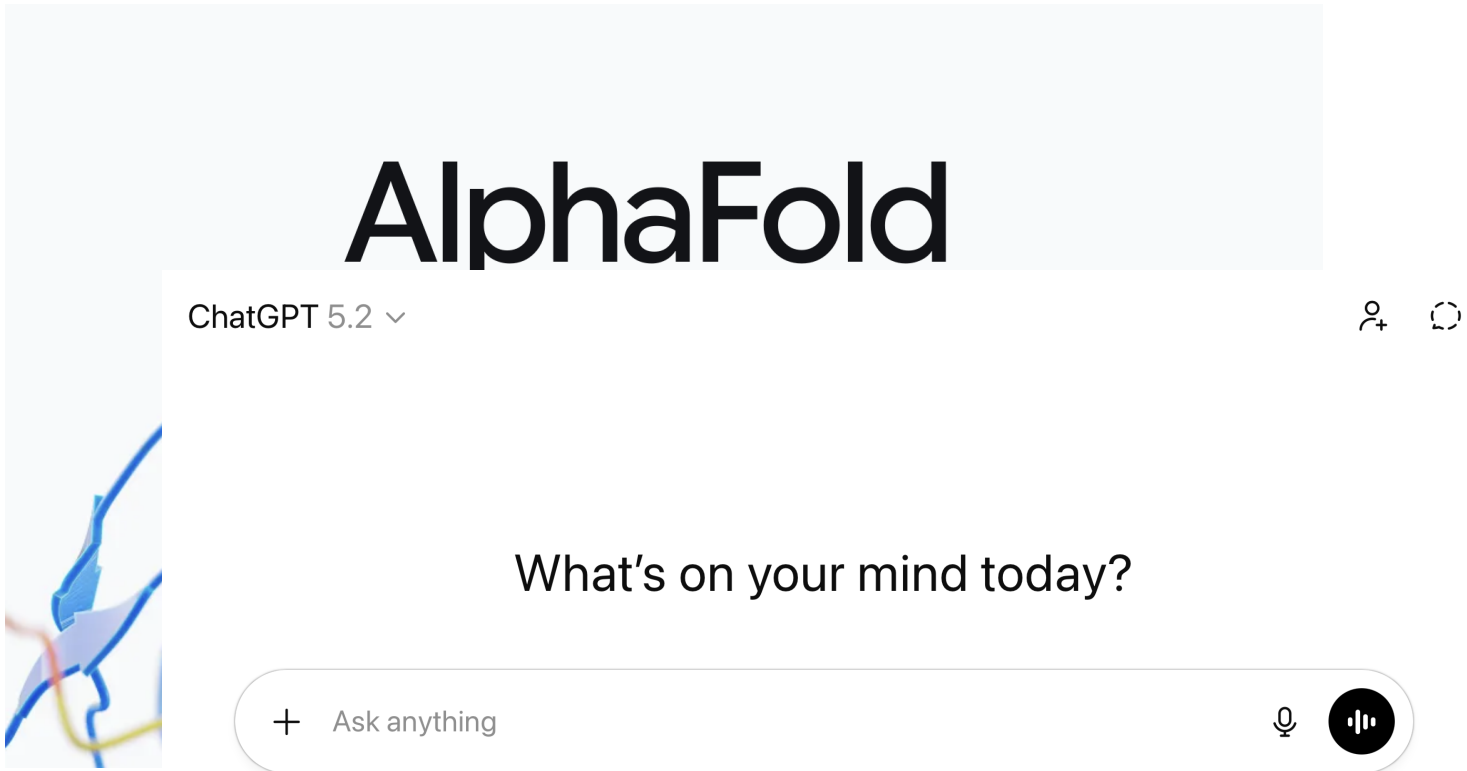

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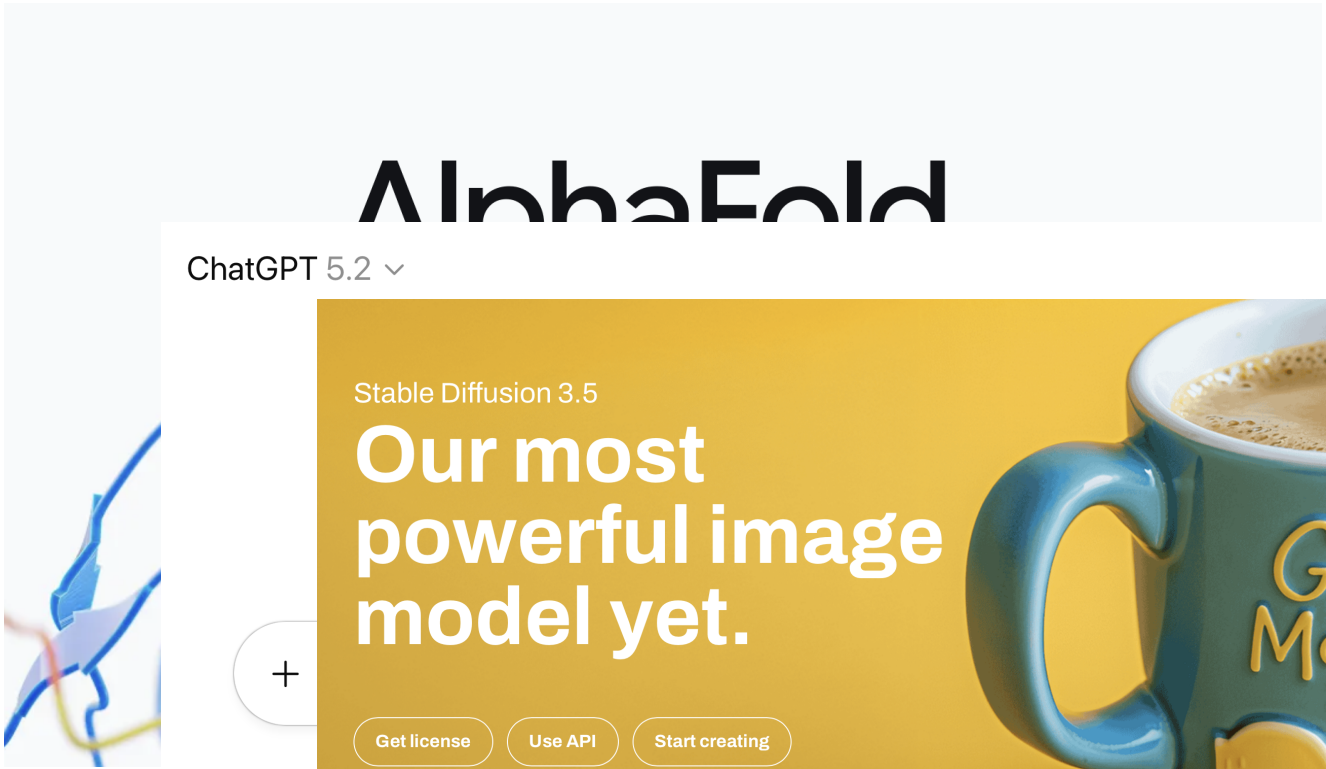
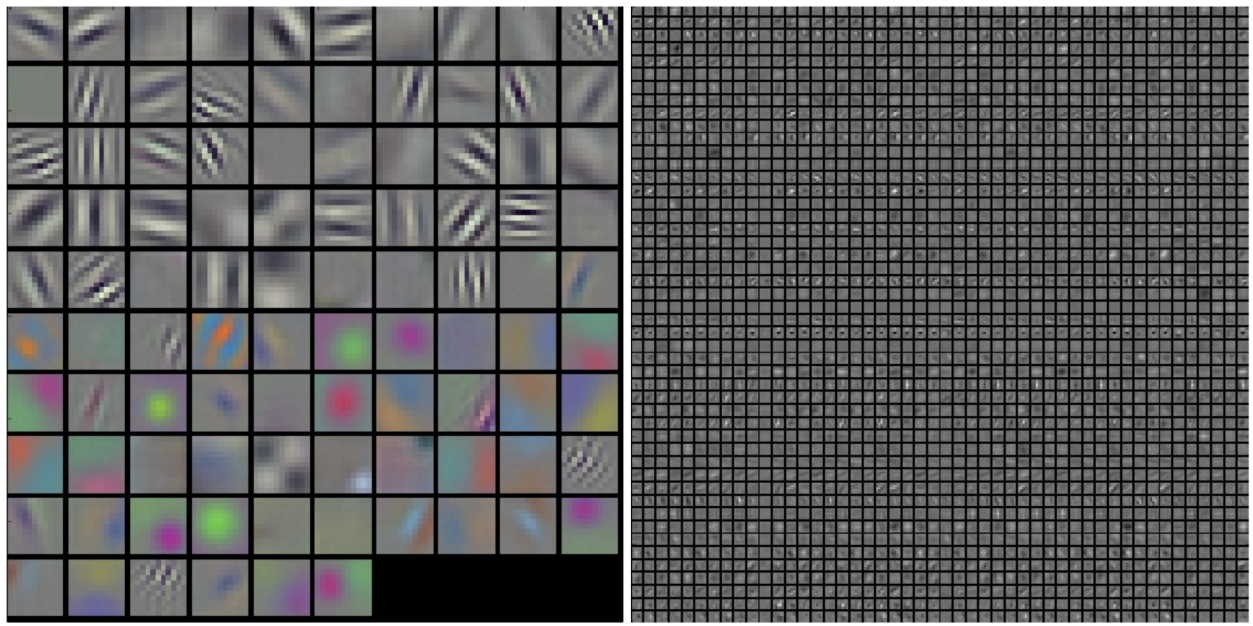


... from learning representations of data



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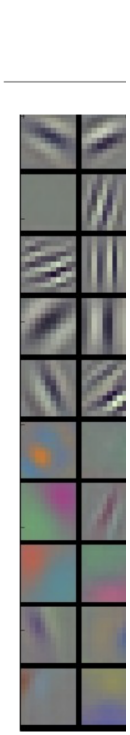
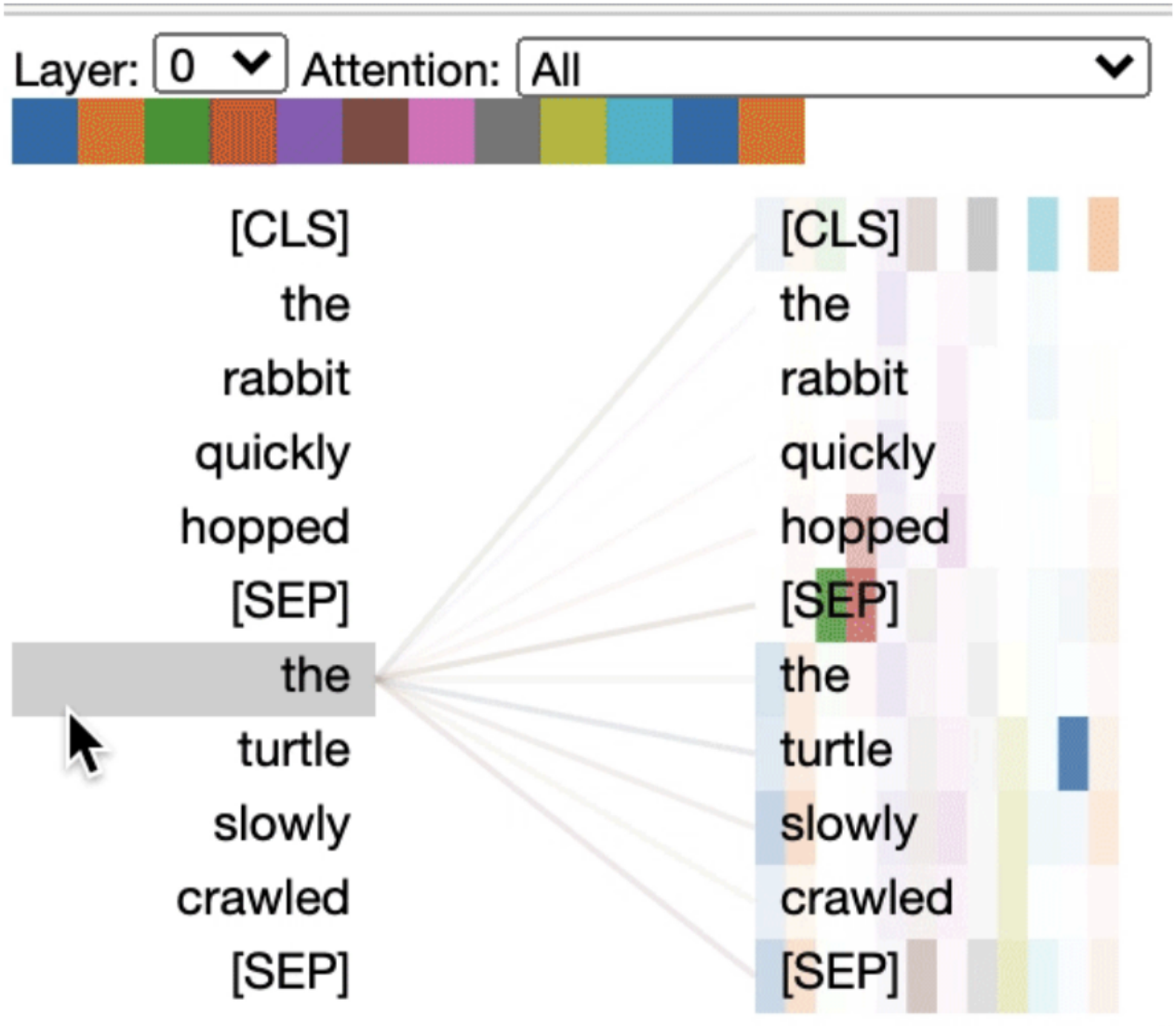
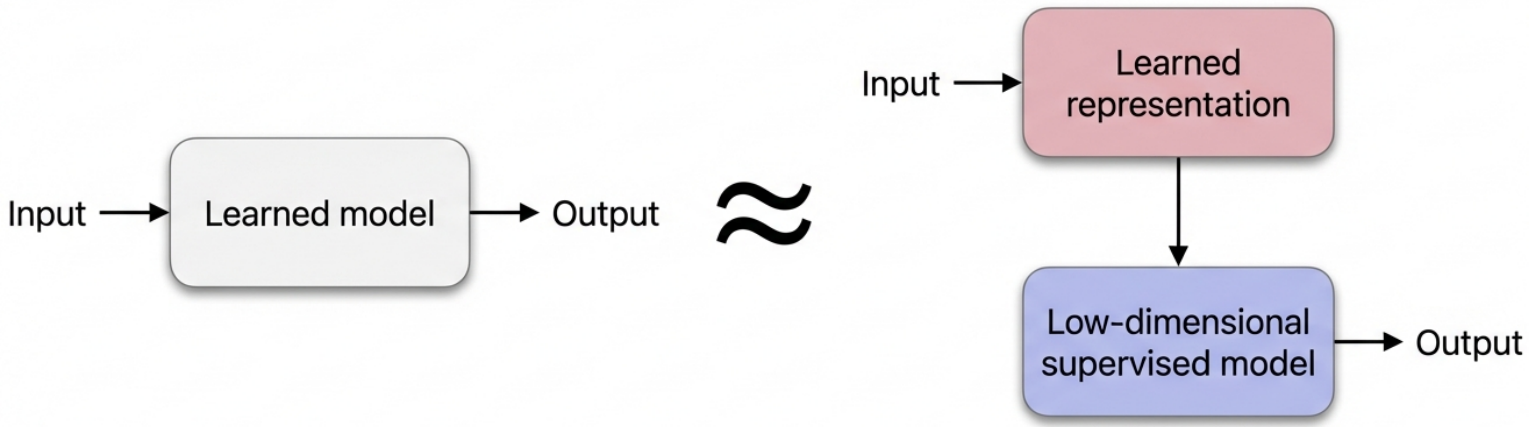




Folklore



First learn representations, then fit a low-dimensional model over those representations!

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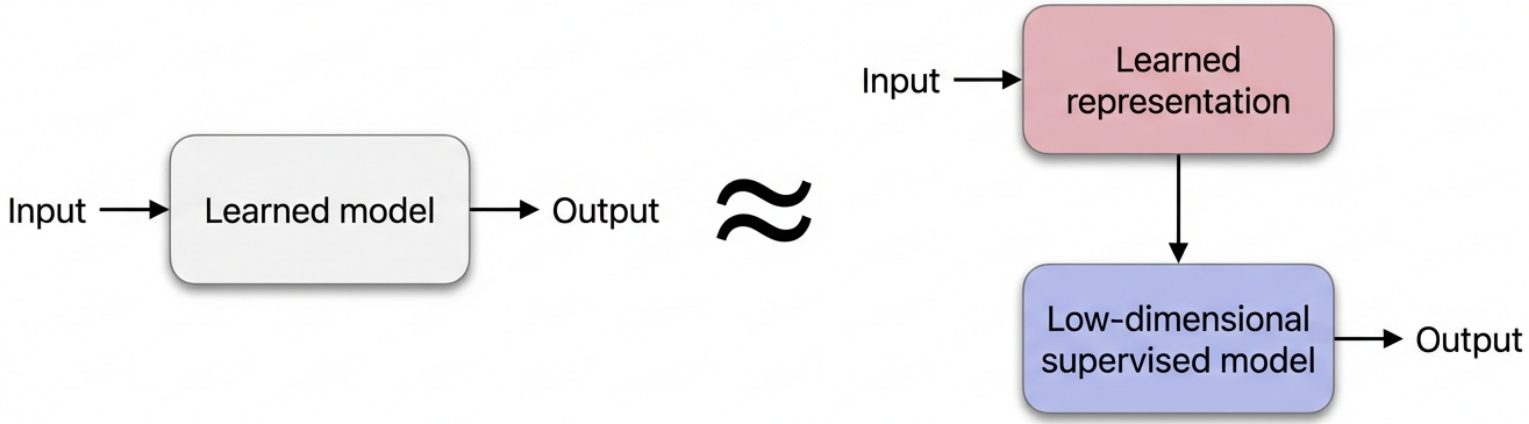

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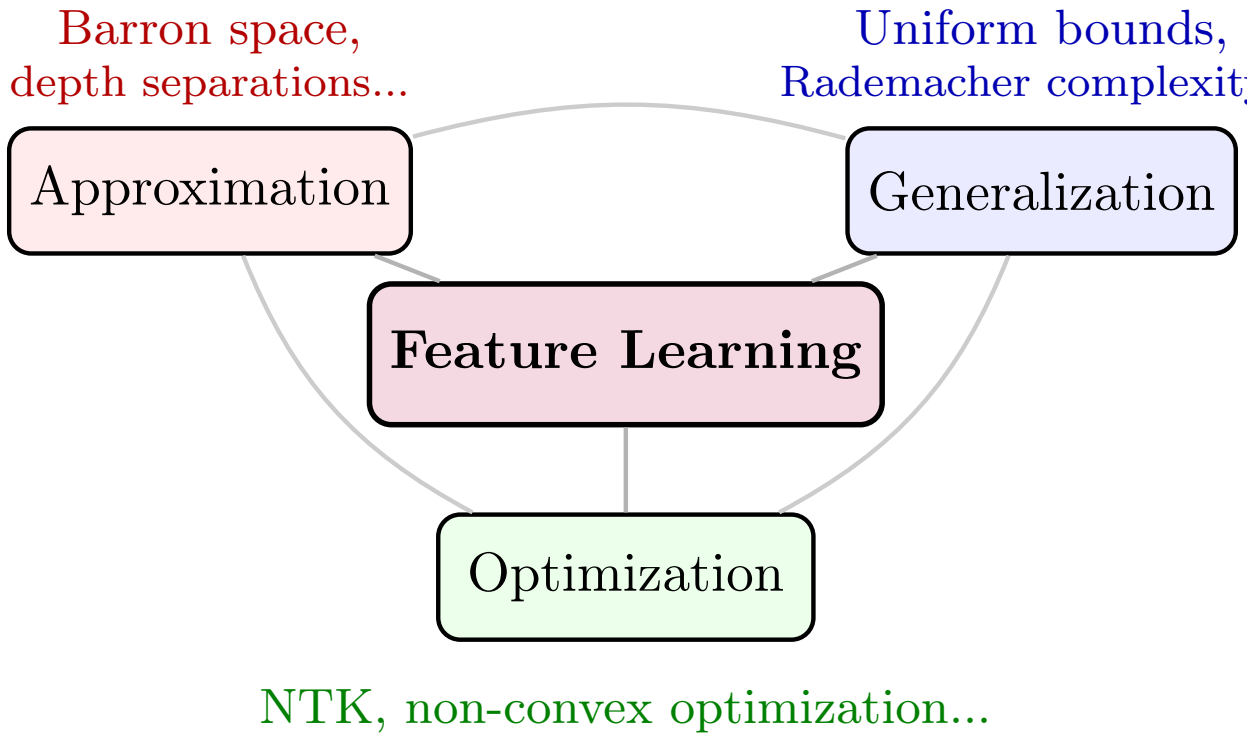
Feature learning

- Feature learning: Learning those representations from data.



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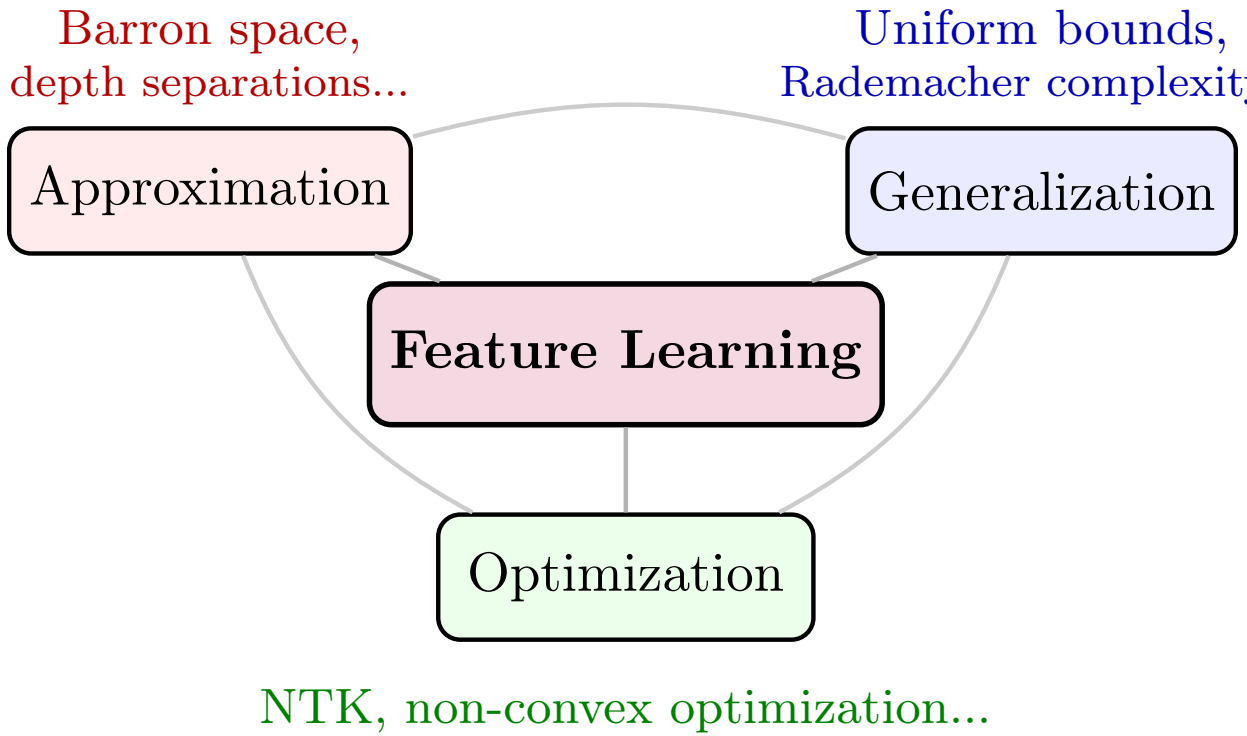

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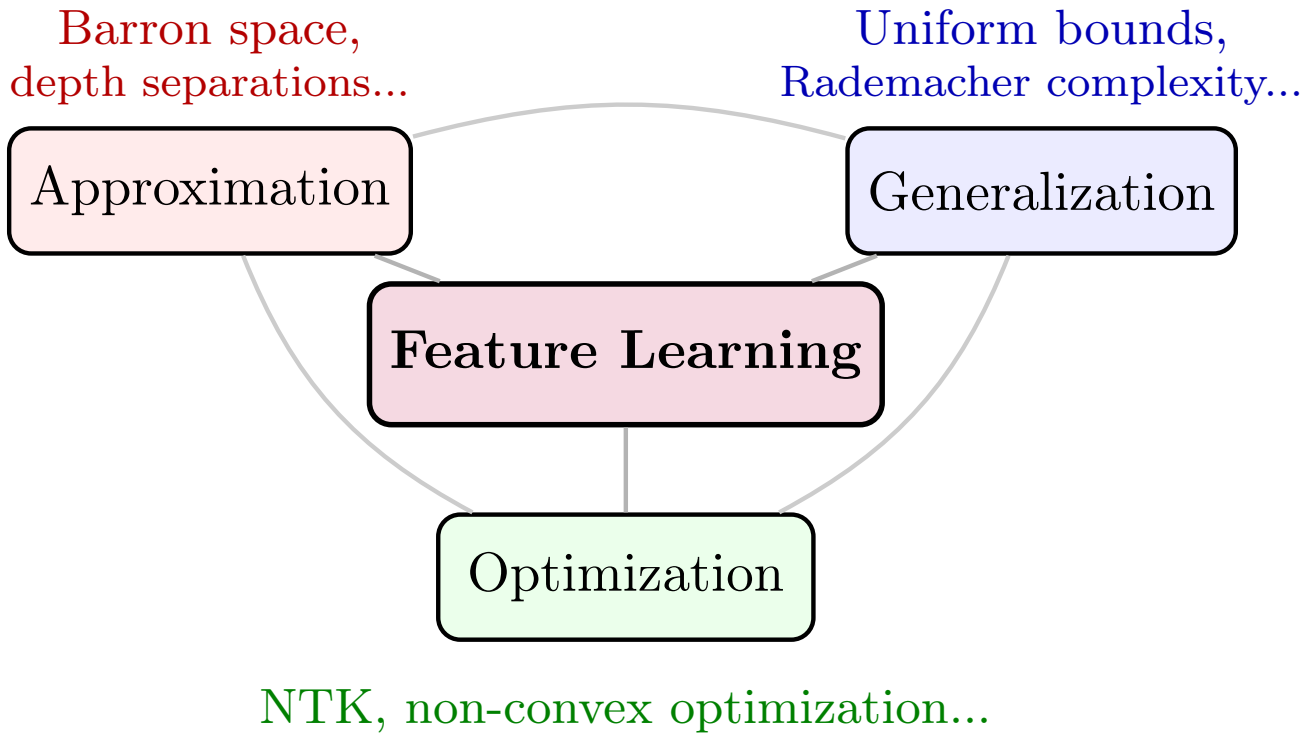
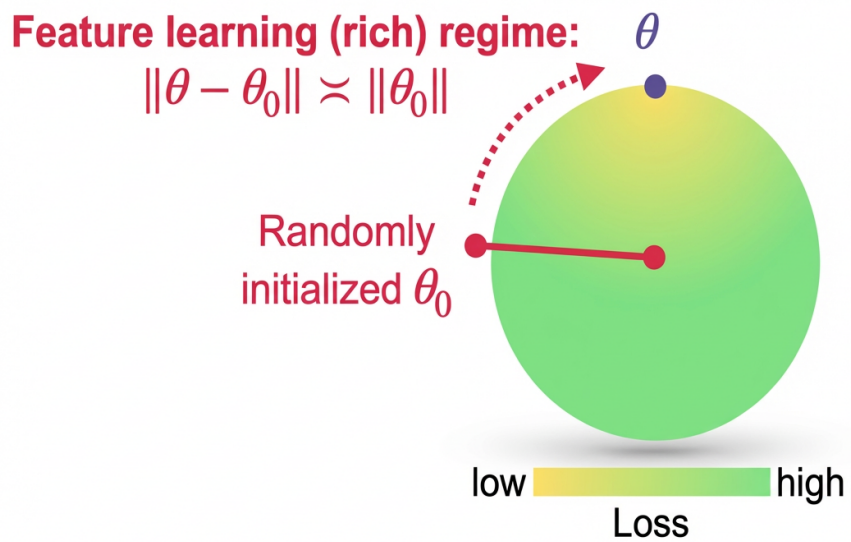


In the feature learning regime, approximation, generalization, and optimization are **entangled** with each other.

Feature learning: not NTK/RF kernel regime

- Consider a neural network $\mathsf{f} : \mathcal{X} \times \mathbb{R}^{\mathsf{D}} \to \mathbb{R}$ that takes input $\mathbf{x} \in \mathcal{X}$ and a parametrization $\boldsymbol{\theta} \in \mathbb{R}^{\mathsf{D}}$ and outputs a scalar.



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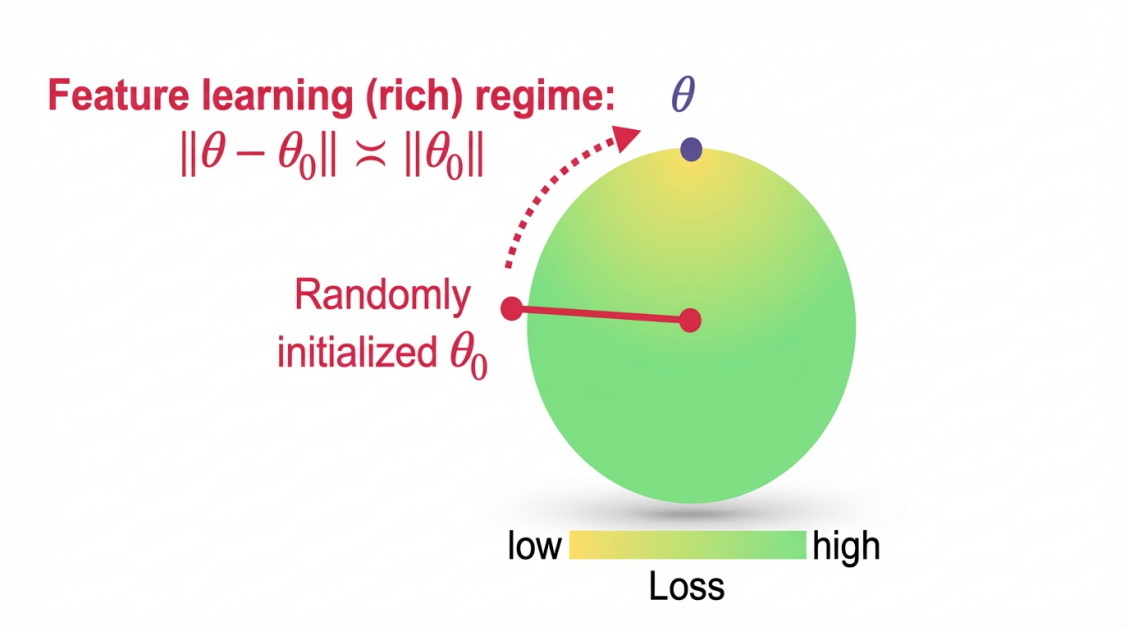

- Kernel/NTK/Lazy training regime: $\|\boldsymbol{\theta} - \boldsymbol{\theta}_0\| \ll \|\boldsymbol{\theta}_0\|$.

Research questions

We aim to answer the following questions:

- Formalize 'feature learning'; a proper mathematical model.
- (Optimization) How models learn features through gradient descent? Understand the **loss landscape and training dynamics**.
- (Generalization) The required **sample size** to learn features. How does this scale with target task, loss function, activation, etc.?

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Outline

Multi-index models

Consider multi-index models as our targets for feature learning.

Setup: Observe n i.i.d. samples $(x_i, y_i)_{i \le n}$:

- Covariates: $x_i \sim \mathsf{N}(0, I_d)$ (high-dimensional, no structure)
- Responses depend on a low-dimensional projection:

$$y_i = h(\Theta_*^\top x_i, \varepsilon_i), \quad \varepsilon_i \sim \mathsf{N}(0,1)$$

- $\Theta_* \in \mathbb{R}^{d \times k}$ $(k \ll d)$
- $h : \mathbb{R}^{k+1} \to \mathbb{R}$ is the link function.

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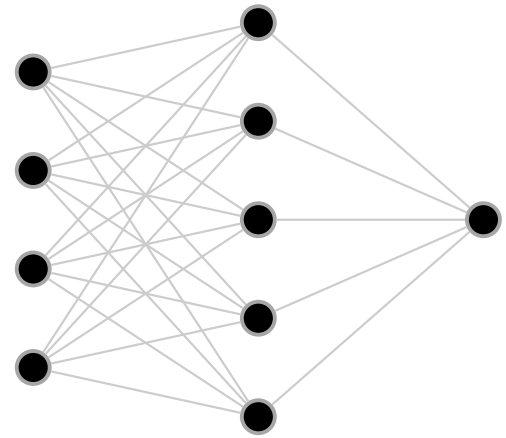
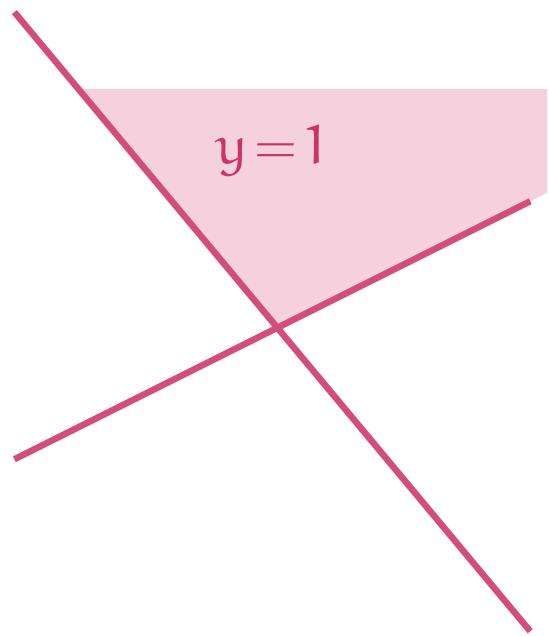
Examples of multi-index models

- **Single-index** $(k = 1)$:
  (e.g., phase retrieval) $y = (\theta_*^\top x)^2$
- **Neural networks** $(O(1)$ neurons$)$:
  $y = \sum_{j=1}^k a_j \sigma(\theta_{*j}^\top x) + \varepsilon$
- **Intersection of halfspaces**:
  $y = \prod_{j=1}^k 1_{\{\theta_{*j}^\top x > 0\}}$
- **Polynomials** on $O(1)$ directions:
  $y = p(\Theta_*^\top x)$





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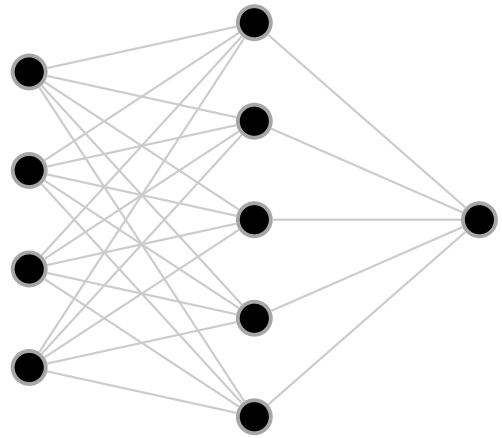

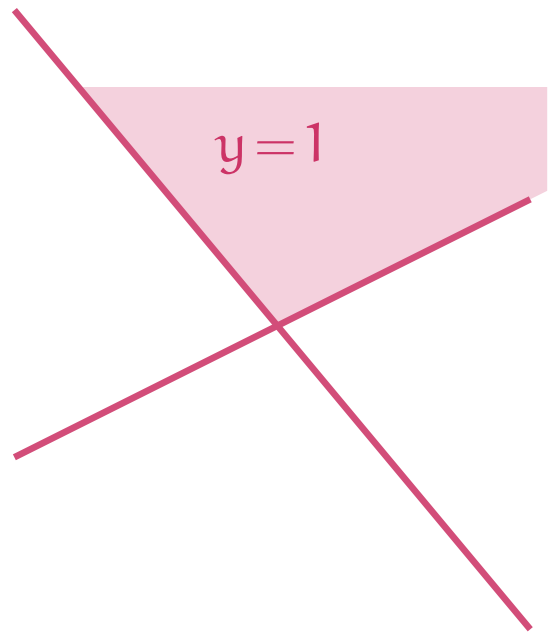

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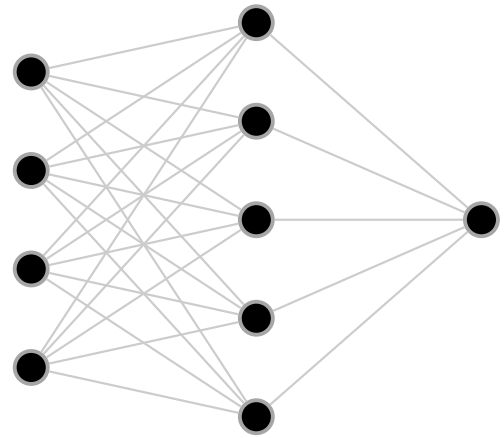

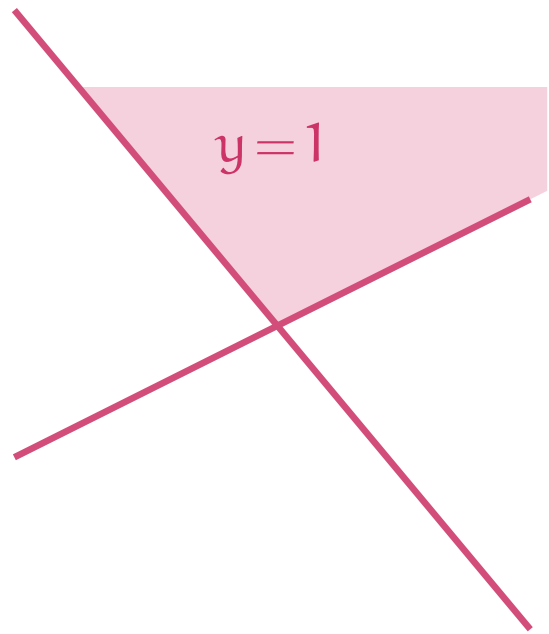

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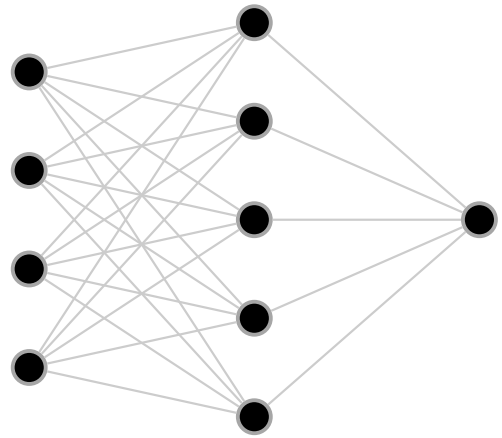

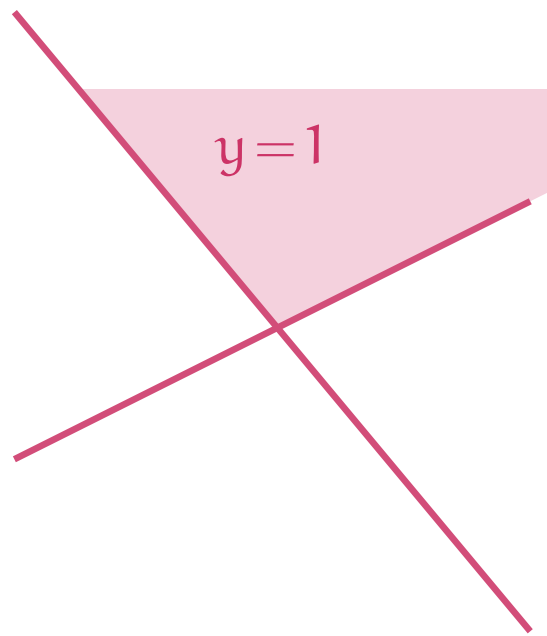

The learning problem

Feature learning = Learning the latent span($\boldsymbol{\Theta}_*$)

Question: How many samples do we need to perform feature learning?

- Simple enough to be tractable mathematically
- Complex enough that NTK/RF/KRR cannot learn[1]

Information-theoretic answer: $n = \Theta(d)$ (counting degrees of freedom) [Barbier, Krzakala, Macris+ '19], [Aubin, Maillard, Barbier+ '19]

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Prior work: Learning multi-index models

Insight: There exist sharp **phase transitions** in $\delta = n/d$.

- **Statistical threshold δ_{IT}:**
  Below δ_{IT}, learning is information-theoretically impossible.

- **Algorithmic threshold δ_{alg}:**
  Below δ_{alg}, no polynomial-time algorithm can learn Θ_*.

Gap: Often $\delta_{\mathsf{IT}} < \delta_{\mathsf{alg}}$ — computational hardness

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Neural Networks? (we want an analogous δ_{NN})

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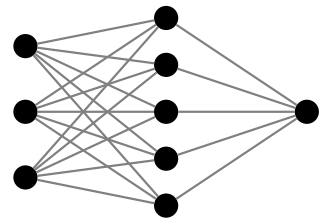
Neural network setup

Two-layer neural network:

$$f_\Theta(x) = \frac{1}{m} \sum_{j=1}^{m} a_j \sigma(\theta_j^\top x + b_j)$$



- $\Theta = [\theta_1, \ldots, \theta_m] \in \mathbb{R}^{d \times m}$: first-layer weights
- σ: activation function (e.g., GeLU, ReLU, ...)
- (a_j, b_j): fixed second-layer weights and biases

Training: Only train Θ via gradient descent on empirical risk

$$\text{Risk}(\Theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f_\Theta(x_i))$$

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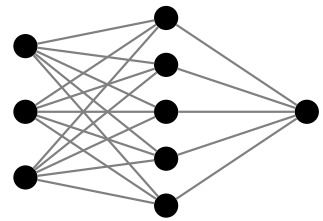

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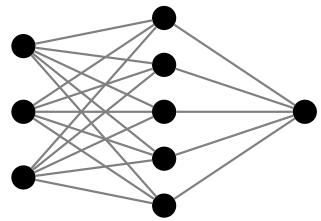

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Training protocol

Full-batch gradient descent:

$$\boldsymbol{\Theta}(t+1) = \boldsymbol{\Theta}(t) - \eta \nabla_{\boldsymbol{\Theta}} \mathsf{Risk}(\boldsymbol{\Theta}(t))$$

Initialization: $\theta_j \overset{\text{i.i.d.}}{\sim} \mathsf{Unif}(\mathbb{S}^{d-1})$

Proportional asymptotics:

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- For generic[2] multi-index models:

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Central question: What is the learning threshold δ_{NN} for gradient descent on neural networks?

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- Target function $\mathsf{h}(\cdot)$,
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We derive an **exact, explicit formula** for computing δ_{NN}:

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1. **Computable:**
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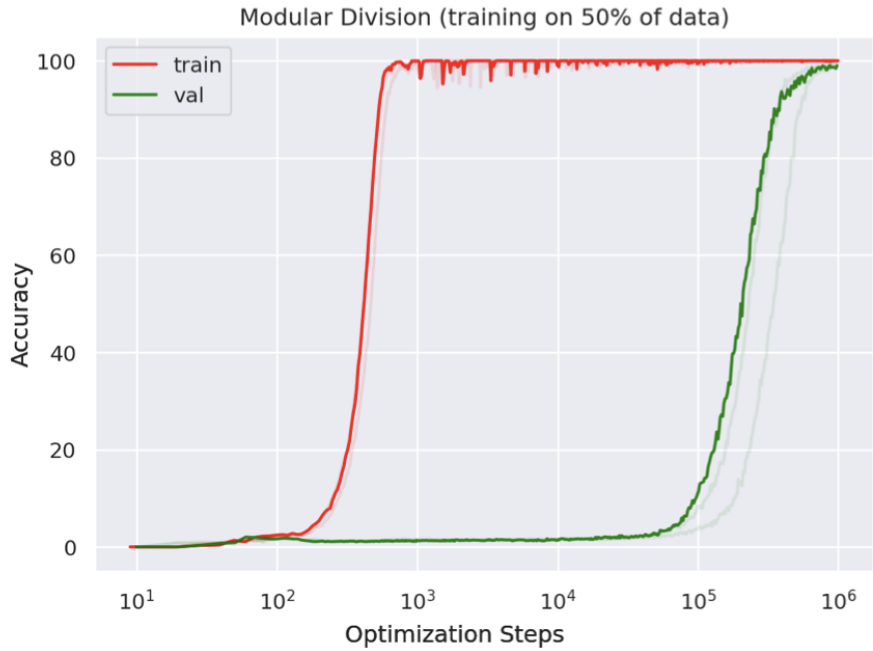
Grokking phenomenon

Grokking: Delayed generalization

- Training error drops quickly
- Test error stays high for long time
- Suddenly: test error drops

Example: Modular division task, trained on transformer architecture.



- Red: train accuracy
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- Gap of $\sim 10^3\times$ in steps

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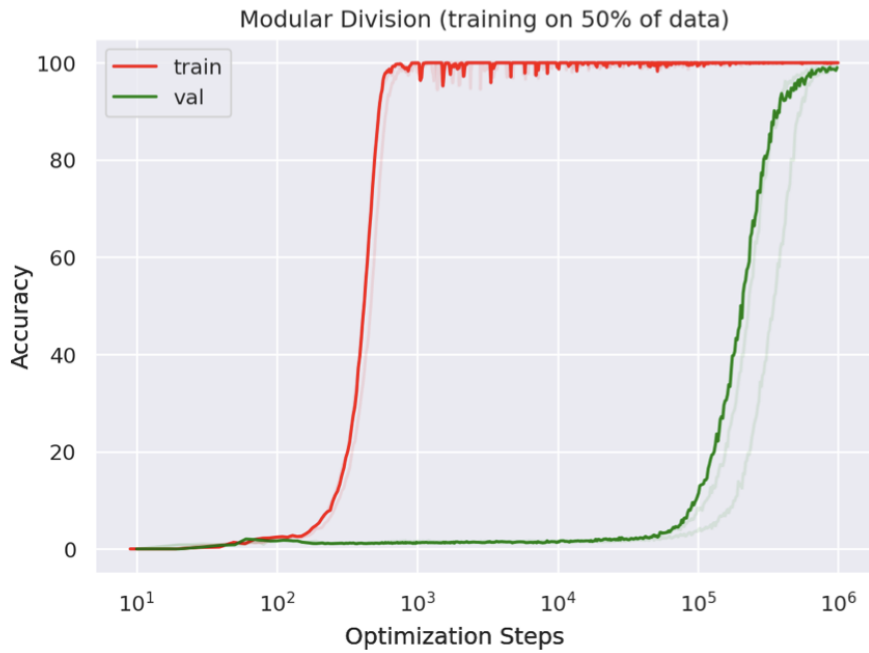

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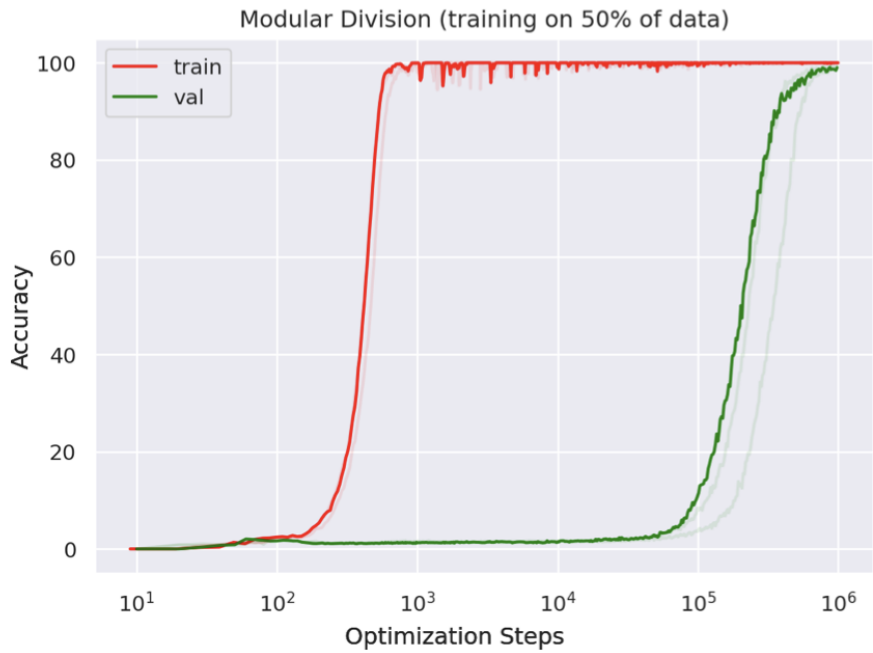

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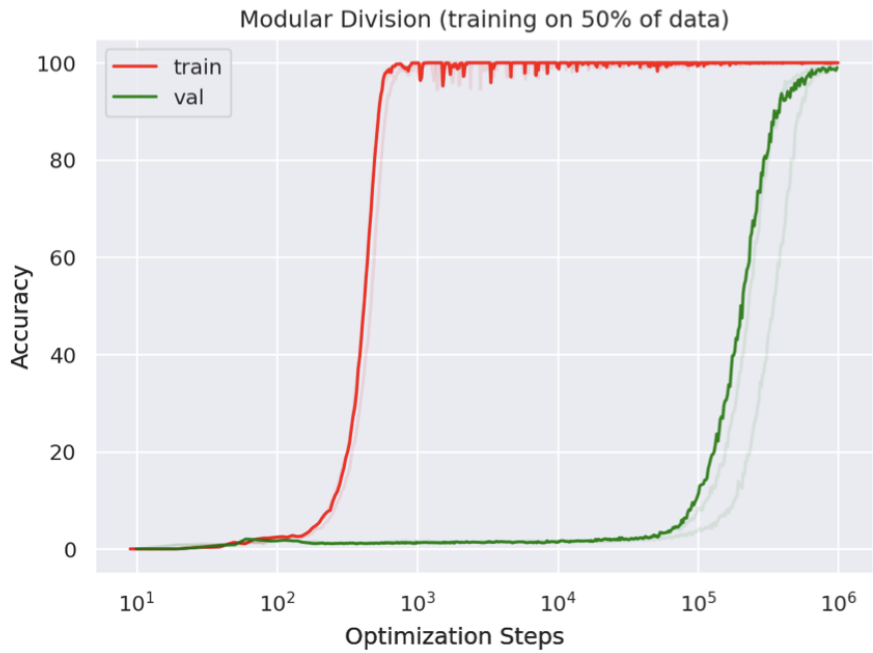

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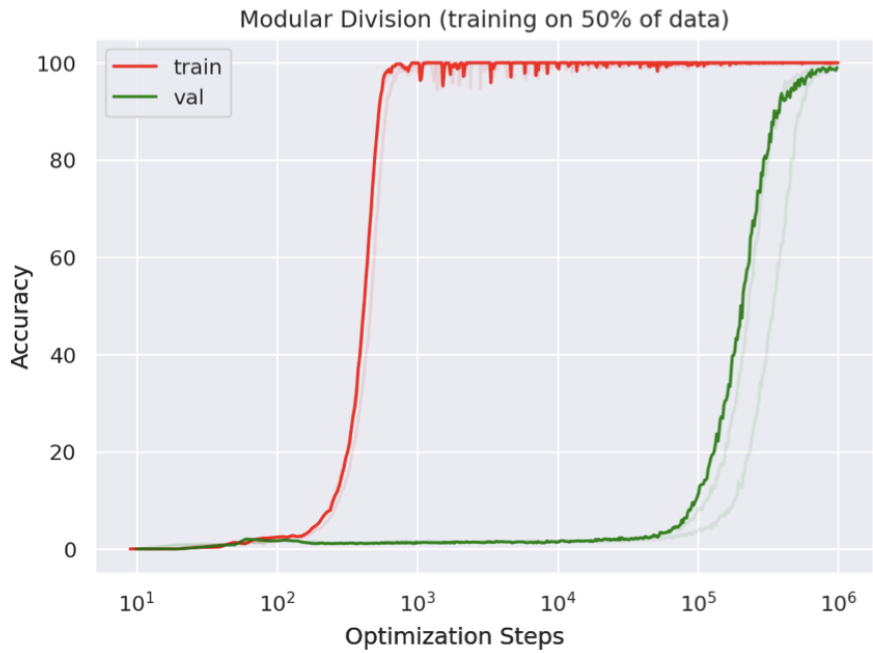

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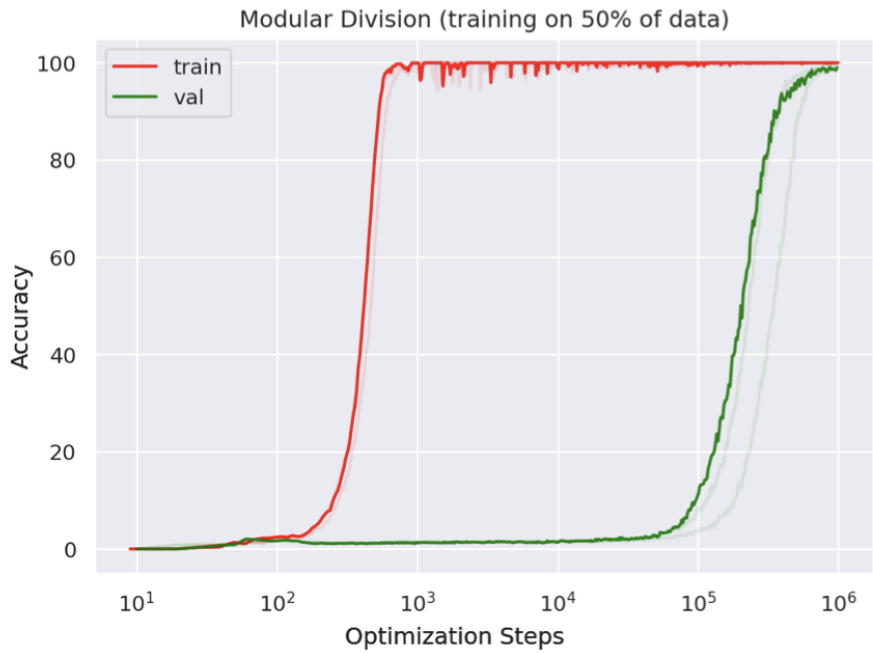

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Demystifying grokking

Our results:

Grokking occurs
when and only when δ is **moderately above** δ_{NN}

- **Moderately above threshold:**
  - Overfit the training data in the first stage of training
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- **Far above threshold** ($\delta \gg \delta_{\mathsf{NN}}$)**:**
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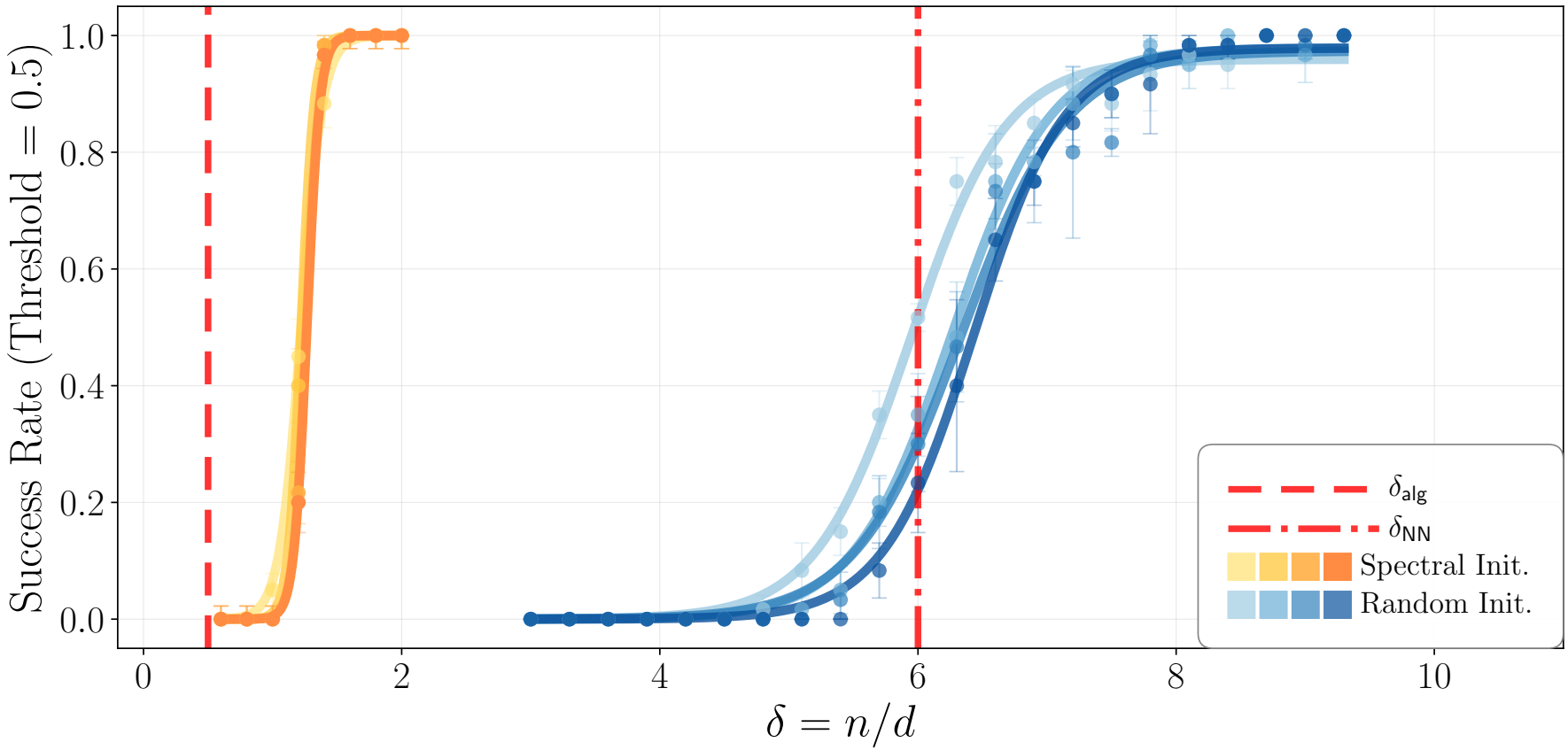
Numerical Illustrations

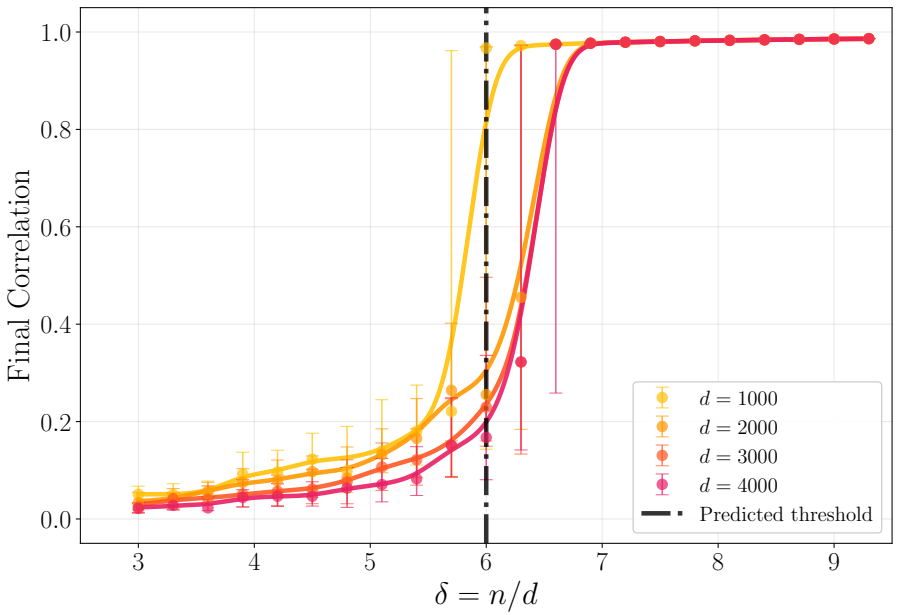
Experiments: Phase transition for feature learning



Single-neuron GeLU network learning phase retrieval ($\mathsf{h}(z) = z^2$).
Success = correlation with θ_* exceeds $1/2$.

Effect of activations

GeLU **activation**



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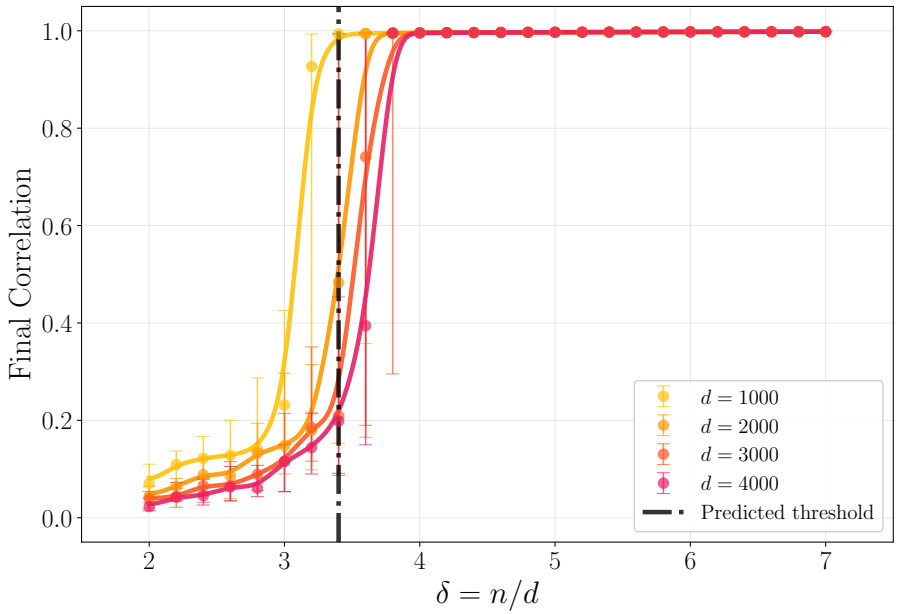

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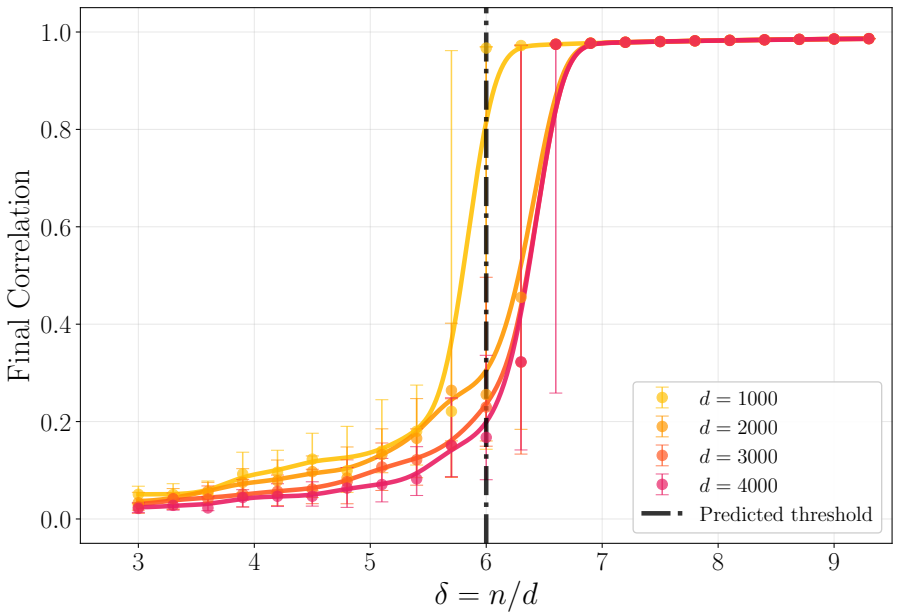

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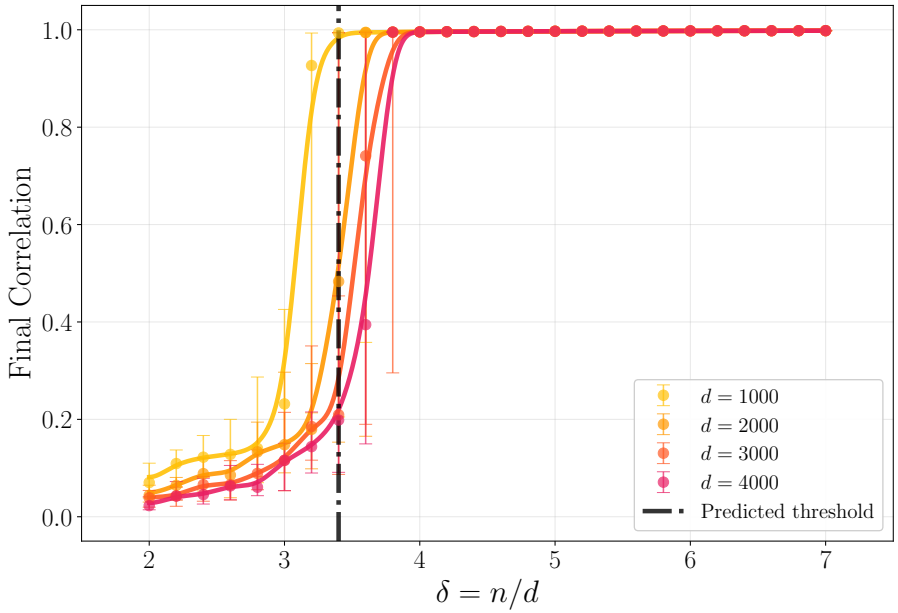

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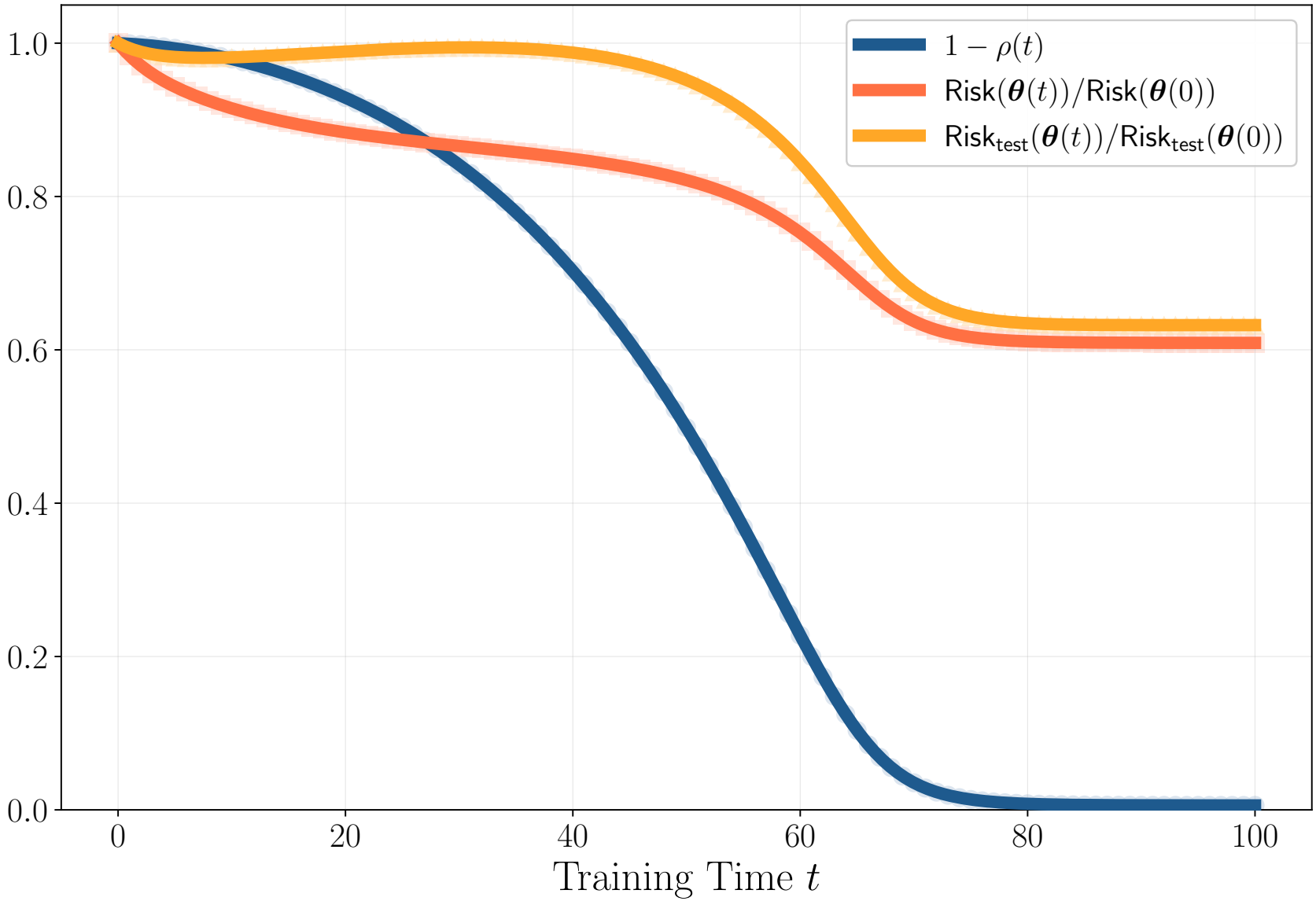
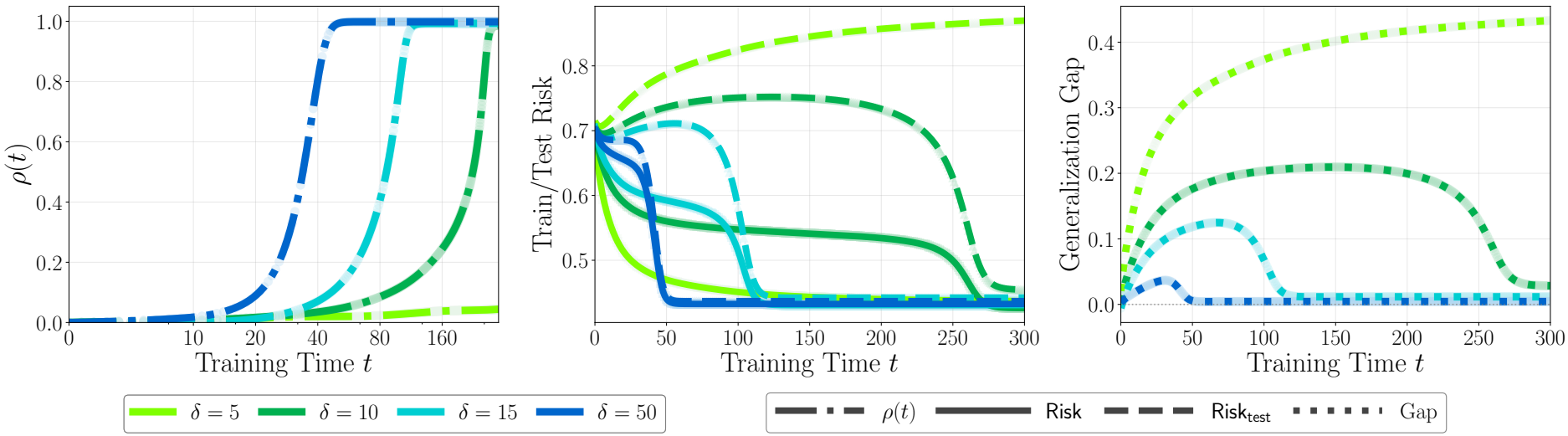


GeLU neuron, phase retrieval, $\mathsf{d} = 5000$, $\delta = 17.5$ (above $\delta_{\mathsf{NN}} \approx 6$).

Experiment: Grokking phenomenon



GeLU neuron, phase retrieval, $\mathrm{d} = 5000$, $\delta = 5, 10, 15, 50$.

Formal results and Outline of the Proofs

Structural decomposition: Insight

The latent space $\text{span}(\boldsymbol{\Theta}_*)$ decomposes into two parts:

Easy subspace

- Learned from **first-order** info of $\mathrm{h}(\cdot)$
- Gradient descent can pick up linear signal

Hard subspace

- **No first-order** info from $\mathrm{h}(\cdot)$
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Hard subspace: $U \in \mathcal{O}(k, k')$ is a hard orthonormal set if

$$\mathbb{E}\big[\mathcal{T}(y, P_U^{\perp} z, \xi) P_U z\big] = 0, \quad \forall \text{ measurable } \mathcal{T} : \mathbb{R}^{k+2} \to \mathbb{R}$$

where $\xi \sim N(0, 1)$ is independent of (y, z) (recall $y = h(z, \varepsilon)$).

The hard subspace $\mathcal{U}_H := \operatorname{span}(U_H^*)$ is the span of the **maximal hard orthonormal set**.

$\mathcal{U}_E := \mathcal{U}_H^{\perp}$

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Setup: $k = 2$, $y = h(z_1, z_2)$ with h symmetric: $h(z_1, z_2) = h(z_2, z_1)$

Decomposition:

- **Easy direction:** $\mathbf{u}_E = \frac{1}{\sqrt{2}}(+1, +1)^\top$
  - $z_1 + z_2$ has linear signal from y
- **Hard direction:** $\mathbf{u}_H = \frac{1}{\sqrt{2}}(+1, -1)^\top$
  - $z_1 - z_2$ has no linear signal (symmetry!)
  - $\mathbb{E}[z_1 - z_2 \mid y, z_1 + z_2] = 0$

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- Single-index with even $h \Rightarrow$ the only direction is hard
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Hard directions: Not learned in $O(1)$ time

Result: For any fixed t

$$\operatorname*{p-lim}_{n,d\to\infty} \Theta(t)^\top \Theta_* P_{U_H^*} = 0$$

More general: Any estimator computed from $O(1)$ gradient steps is uncorrelated with hard directions.

Tool: Dynamical Mean Field Theory (DMFT)[5]

- Exact characterization of GD in the limit $n, d \to \infty$
- Constructs low-dimensional random vectors $(V(t), \Theta(t))$ that characterizes the dynamics

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Easy directions: Learned in $O(1)$ time

The network weakly learns the easy subspace within $O(1)$ iterations[6]:

There exists $\varepsilon_0 > 0$, $t = O(1)$ such that

$$\lim_{n,d\to\infty} \mathbb{P}\left(\left|\left|\boldsymbol{\Theta}(t)^\top \boldsymbol{\Theta}_* U_E^*\right|\right| \geq \varepsilon_0\right) = 1$$

Intuition:

- Easy directions have linear signal in the gradient
- Standard gradient descent picks up this signal

The learning bottleneck is the hard directions.

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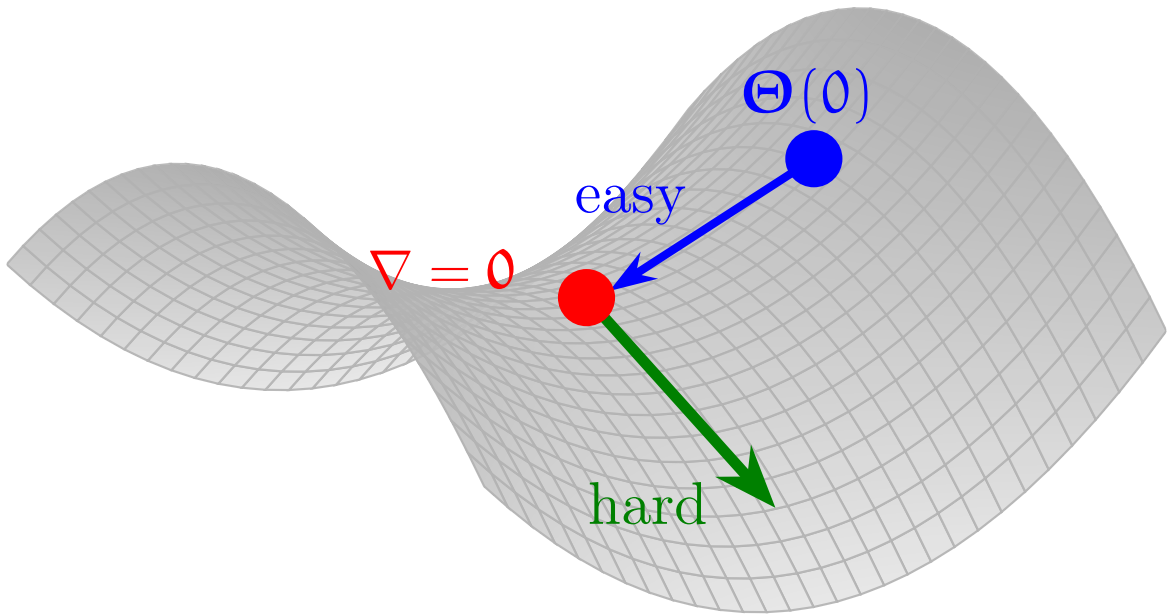
Learning hard directions: The problem

Problem: No linear signal for hard directions

$\Rightarrow$ First-order methods approach a **saddle point**.



Learning hard directions: The solution

Solution: **Use second-order information to escape saddle**

- Study the (rescaled) Hessian

$$\mathbf{H}(t) := m\nabla^2 \mathsf{Risk}(\boldsymbol{\Theta}(t))$$

  along GD trajectory
- Look for **negative eigenvalues** of the Hessian with eigenvectors aligned with hard subspace
- Such eigenvectors directions enable **escape from saddle** $\Rightarrow$ learning those hard directions

Question: When does the Hessian have **informative descent directions** after $O(1)$ iterations?

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Hessian structure

Case $m = 1$ (single neuron): $\mathbf{H}(t) \in \mathbb{R}^{d \times d}$

$$\mathbf{H}(t) = \frac{1}{n} \sum_{i=1}^{n} g(y_i, \theta(t)^\top x_i) x_i x_i^\top$$

where
$g(y, z) = a^2 \ell''(y, a\sigma(z + b))\sigma'(z + b)^2 + a\ell'(y, a\sigma(z + b))\sigma''(z + b)$

Case $m \gg 1$ (wide network): $\mathbf{H}(t) \in \mathbb{R}^{md \times md}$

- Block structure with m^2 blocks of size $d \times d$
- For convex loss: well-approximated by block-diagonal $\mathbf{H}_{\text{diag}}(t)$
- Each block $a_j \mathbf{H}_j(t)$ where $\mathbf{H}_j(t) = \frac{1}{n} \sum_{i=1}^{n} g(y_i, \Theta(t)^\top x_i; j) \cdot x_i x_i^\top$
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Main result: Hessian phase transition

(Stated for $m \gg 1$; similar result holds for $m = 1$)

Results (informal): Under the propotional asymptotic, there exist thresholds δ_j^* for each block j:

If $\delta > \delta_j^*$: For t large enough,

- $H_j(t)$ has a **negative outlier eigenvalue** below the bulk
- The corresponding eigenvector is **correlated with hard subspace**

If $\delta < \delta_j^*$: For all large enough t,

- No eigenvector of $H_j(t)$ is correlated with hard subspace

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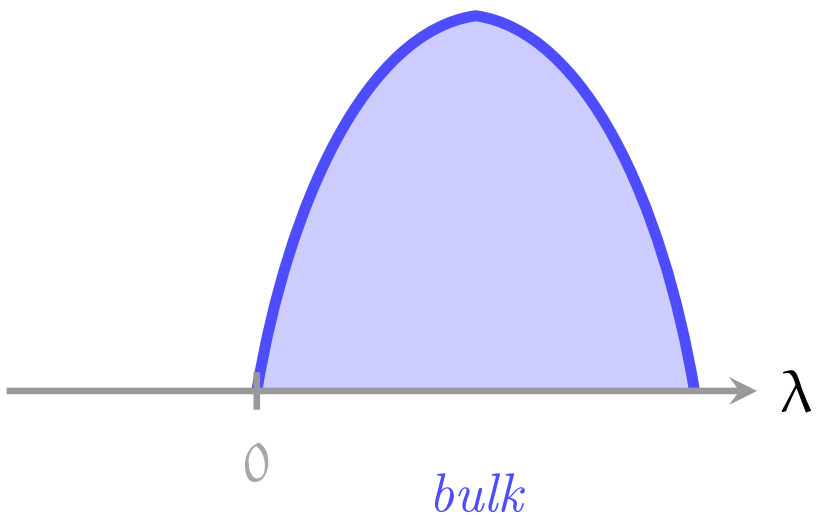
Spectrum of the Hessian

$\delta < \delta_{NN}$



No informative direction

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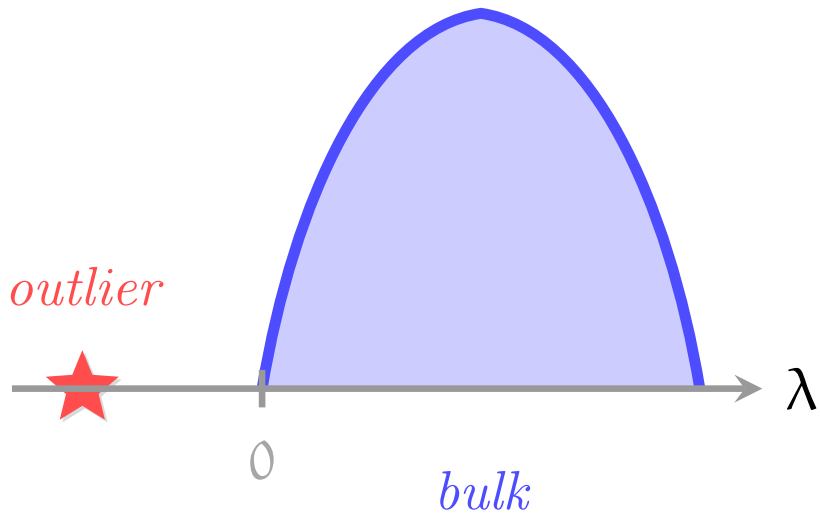

Descent direction → hard subspace!

DMFT: Evolution equations

Next, we state the formula for computing δ_{NN}.
In order to do so, we need to introduce **Dynamical Mean Field Theory (DMFT)** [7].

Goal: Characterize gradient descent dynamics as $n, d \to \infty$ via low-dimensional random variables.

$$(V(t), V_*) \in \mathbb{R}^m \times \mathbb{R}^k$$

$$V(t) = W(t) - \frac{1}{\delta} \sum_{s=0}^{t-1} R_\theta(t,s) F(V(s), V_*, \varepsilon), \quad W \sim \mathsf{GP}(0, C_\theta)$$

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DMFT: Convergence

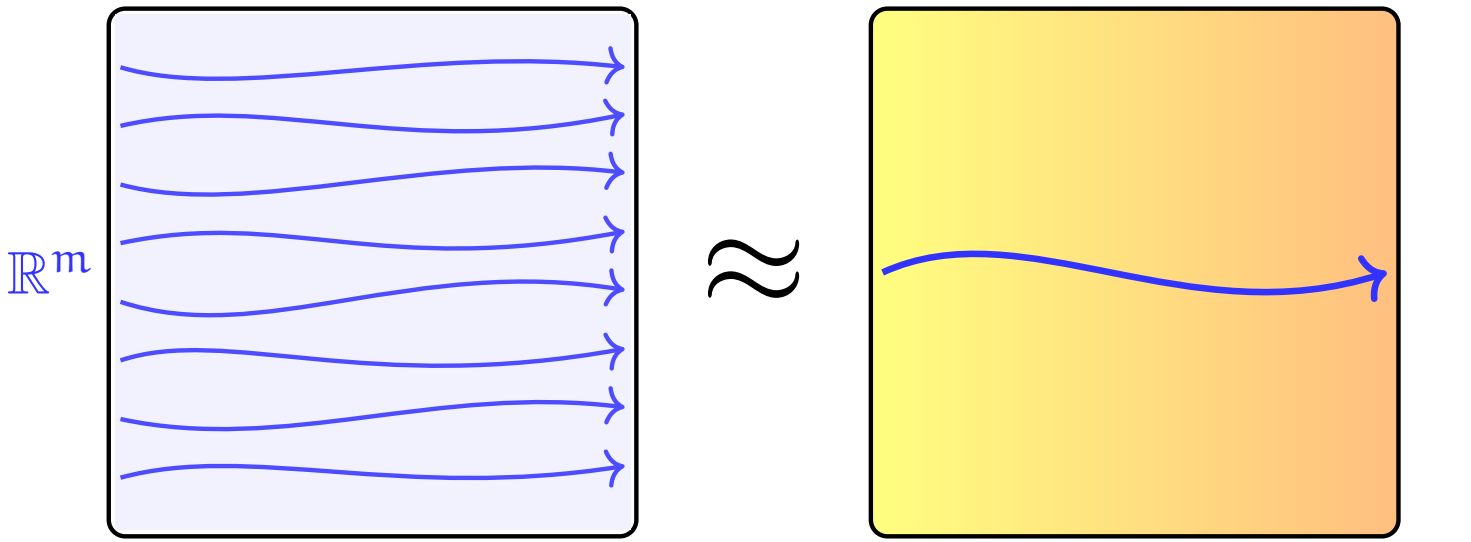
For test function ϕ,

$$\frac{1}{n}\sum_{i=1}^{n}\phi(\boldsymbol{\Theta}(t)^\top \mathbf{x}_i, \boldsymbol{\Theta}_*^\top \mathbf{x}_i, \varepsilon_i) \xrightarrow{p} \mathbb{E}\big[\phi(V(t), V_*, \varepsilon)\big]$$

$$\frac{1}{d}\sum_{i=1}^{d}\phi(\sqrt{d}\boldsymbol{\Theta}(t)_i, \sqrt{d}\boldsymbol{\Theta}_{*i}) \xrightarrow{p} \mathbb{E}\big[\phi(\Theta(t), \Theta_*)\big]$$

Remark: Formulas scale with k, m and t, **not** with n and d

DMFT: Main idea



d particles in $\mathbb{R}^m$ one part. + noise + memory

'Gaussian' approximation + Symmetries

$\Rightarrow$ Integral equations for memory + response kernels

Bulk spectrum of the Hessian

Hessian block: $\mathbf{H}_j(t) = \frac{1}{n}\sum_{i=1}^{n} g(y_i, \boldsymbol{\Theta}(t)^\top \mathbf{x}_i; j) \cdot \mathbf{x}_i \mathbf{x}_i^\top$

Limiting spectral distribution: $\mu_{n,d}^j(t) \Rightarrow \mu_\infty^j(t)$ with $\alpha_t^j(z)$ the Stieltjes transform of $\mu_\infty^j(t)$.

Stieltjes transform: For $z \in \mathbb{C}^+$, $\alpha_t^j(z)$ is the unique solution of

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Hessian block: $\mathbf{H}_j(t) = \frac{1}{n}\sum_{i=1}^{n} g(y_i, \boldsymbol{\Theta}(t)^\top \mathbf{x}_i; j) \cdot \mathbf{x}_i \mathbf{x}_i^\top$

Limiting spectral distribution: $\mu_{n,d}^j(t) \Rightarrow \mu_\infty^j(t)$ with $\alpha_t^j(z)$ the Stieltjes transform of $\mu_\infty^j(t)$.

Stieltjes transform: For $z \in \mathbb{C}^+$, $\alpha_t^j(z)$ is the unique solution of

$$z + \frac{1}{\alpha_t^j(z)} = \delta \cdot \mathbb{E}\left[\frac{G_t^j}{\delta + G_t^j \alpha_t^j(z)}\right]$$

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Edge and outlier equations

Left edge: $$A_t^j := \frac{\delta}{(-\inf(\mathrm{supp}(\mathrm{Law}(G_t^j)))) \vee 0}$$

$$c_j(t) := \sup_{\alpha \in (0, A_t^j)} \left\{ -\frac{1}{\alpha} + \delta \cdot \mathbb{E}\left[\frac{G_t^j}{\delta + G_t^j \alpha} \right] \right\}$$

Outlier equation: For $z < \min(0, c_j(t))$,

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$$\delta_j^*(t) := \inf\{\delta > 0 : \text{outlier eq. has solution } z < \min(0, c_j(t))\}$$

$$\delta_j^*(\infty) := \lim_{t\to\infty} \delta_j^*(t)$$

Overall: $$\delta_{NN} := \min_{j\in[m]} \delta_j^*(\infty)$$

- $\delta > \delta_{NN}$: Hessian has informative descent direction $\Rightarrow$ learn hard subspace
- $\delta < \delta_{NN}$: No informative direction $\Rightarrow$ cannot learn

Remark: For $m = 1$, similar formulas hold with G_t^j replaced by $G_t = \ell''\sigma'^2 + \ell'\sigma''$.

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Grokking explanation

Setup: (We assume for now) only hard directions to learn, $\delta > \delta_{\mathsf{NN}}$

Stage 1: $t = O(1)$

- Cannot learn hard directions (no linear signal)
- But $n/d = \delta$ is finite $\Rightarrow$ **overfits a bit training data**
- Train loss $\ll$ Test loss (generalization gap)

Stage 2: Saddle escape happens

- Since $\delta > \delta_{\mathsf{NN}}$: Hessian **develops informative outlier**
- Eventually **learns hard directions**
- Test loss drops $\Rightarrow$ **Predictable grokking!**

No grokking when $\delta \gg \delta_{\mathsf{NN}}$:

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Proof techniques

Our proofs utilize three main ingredients:

1. **Dynamical Mean Field Theory (DMFT)**
   - Tracks the evolution of GD in the first stage of training
2. **Gaussian conditioning**
3. **Random Matrix Theory (RMT)**
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▷ Proofs are mathematically involved but conceptually straightforward. Detailed proof sketch in the appendix.

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Discussion

Conclusion

Main contributions:

1. **Precise threshold δ_{NN}** for feature learning (the first hard direction) via gradient descent on two-layer NNs
   - ▻ Depends on target, loss, activation, width, initialization
   - ▻ Efficiently computable from problem setup
2. **Spectral mechanism:** Learning hard directions $\Leftrightarrow$ negative outliers of Hessian aligned with hard subspace
3. $\delta_{\mathsf{NN}} > \delta_{\mathsf{alg}}$ in general; gap depends on architecture and training
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Remarks

Multi-index models as a testbed

- Multi-index models are an excellent mathematical framework for understanding feature learning. It captures the essential challenge: learning low-dimensional structure from high-dimensional data.
- Simple enough for performing precise mathematical arguments, complex enough to rule out kernel methods and observe non-trivial phenomena observed in practice (feature learning, grokking, etc).

Beyond multi-index models

- hierarchical/compositional targets

$$y = g(p_1(\boldsymbol{x}), \ldots, p_k(\boldsymbol{x})) \text{ or } y = g_k \circ \cdots \circ g_1(\boldsymbol{x})$$

- Interesting in capturing hierarchical feature learning in deep networks

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Thanks for listening!

Questions?

arXiv:2602.01434

Proof sketch: Setup

(WLOG consider $m \gg 1$; the case $m = 1$ is similar)

Object of interest: Hessian diagonal block

$$H_j(t) = \frac{1}{n} \sum_{i=1}^{n} g(y_i, \Theta(t)^\top x_i; j) \cdot x_i x_i^\top = X^\top G_j(t) X$$

Intuition: y_i only depends on **few directions** $\Theta_*^\top x_i$
$\Rightarrow$ $G_j(t)$ carries low-rank informative signal $\Rightarrow$ expect outliers

Why is this hard? Not a standard spiked random matrix

- $\Theta(t)$ depends on (X, y) through GD updates
- Complex nonlinear dependence $\Rightarrow$ standard RMT does not work

Key insight: Although nonlinear, each GD update is **linear in X**

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Proof sketch: Step 1 – Gaussian conditioning

Gaussian conditioning decomposition:

$$\mathbf{X} \overset{d}{=} \mathbf{P}_{\mathbf{F}}^{\perp} \mathbf{X}_{\text{new}} \mathbf{P}_{\boldsymbol{\Theta}}^{\perp} + \mathbf{X} \mathbf{P}_{\boldsymbol{\Theta}}$$

- $\mathbf{X}_{\text{new}}$: fresh i.i.d. $\mathsf{N}(0,1)$ matrix, **independent** of training data
- $\mathbf{P}_{\boldsymbol{\Theta}}$, $\mathbf{P}_{\mathbf{F}}$: projectors onto parameter/gradient subspaces

This technique has been extensively studied in AMP literature[8].

Result:

$$\mathbf{H}_j(t) \overset{d}{=} \mathbf{X}_{\text{new}}^{\top} \mathbf{G}_j(t) \mathbf{X}_{\text{new}} + \text{finite-rank perturbation}$$

$\Rightarrow$ Bulk follows **generalized Marchenko-Pastur law**
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Proof sketch: Step 2 – Outlier detection

From Step 1: $\mathbf{H}_j(t) \overset{d}{=} \mathbf{X}_{\text{new}}^\top \mathbf{G}_j \mathbf{X}_{\text{new}} + \text{finite-rank}$

Woodbury identity: For $A + UCV$,

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Apply to resolvent:

$$(\mathbf{H}_j(t) - zI)^{-1} = R_0(z) - R_0(z) \cdot [\text{low-rank}] \cdot \mathbf{M}_j(z;t)^{-1} \cdot [\text{low-rank}]^\top \cdot R_0(z)$$

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Key: z is an outlier eigenvalue $\Leftrightarrow \det(\mathbf{M}_j(z;t)) = 0$

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$$(\mathbf{H}_j(t) - zI)^{-1} = R_0(z) - R_0(z) \cdot [\text{low-rank}] \cdot \mathbf{M}_j(z;t)^{-1} \cdot [\text{low-rank}]^\top \cdot R_0(z)$$

where $R_0(z) = (\mathbf{X}_{\text{new}}^\top \mathbf{G}_j \mathbf{X}_{\text{new}} - zI)^{-1}$ is the **bulk resolvent**

Key: z is an outlier eigenvalue $\Leftrightarrow \det(\mathbf{M}_j(z;t)) = 0$

$\mathbf{M}_j(z;t)$ is finite-dimensional (size $\sim k + mt$, independent of n, d)

Proof sketch: Step 2 – Outlier detection

From Step 1: $\mathbf{H}_j(t) \overset{d}{=} \mathbf{X}_{\text{new}}^\top \mathbf{G}_j \mathbf{X}_{\text{new}} + \text{finite-rank}$

Woodbury identity: For $A + UCV$,

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Apply to resolvent:

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Proof sketch: Step 2 – Block structure

Concentration: $\mathbf{M}_j(z;t) \xrightarrow{p} M_j^\infty(z;t)$ (deterministic limit)

Fortunately: $M_j^\infty(z;t)$ has **block-diagonal structure**!

$$\det(M_j^\infty(z;t)) = 0 \quad \Leftrightarrow \quad \det(M_{j,H}^\infty) = 0 \text{ or } \det(M_{j,R}^\infty) = 0$$

- $M_{j,H}^\infty$: **Hard block** (size $r \times r$, independent of t)
  $\Rightarrow \det(M_{j,H}^\infty) = 0$ gives our **outlier equation**
- $M_{j,R}^\infty$: **Rest block**
  $\Rightarrow$ Can prove: solutions have **no informative eigenvectors**

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Proof sketch: Step 3 – Eigenvector alignment

Residue formula:

$$\xi\xi^\top = -\frac{1}{2\pi i}\oint_\gamma (H_j(t) - zI)^{-1}\,dz$$

Correlation:

$$\|\Theta_{*H}^\top \xi\|^2 = -\frac{1}{2\pi i}\oint_\gamma \mathrm{Tr}\big(\Theta_{*H}^\top (H_j(t) - zI)^{-1}\Theta_{*H}\big)\,dz$$

Simplification:

- Substitute resolvent expansion from the last step
- $R_0(z)$ analytic inside $\gamma \Rightarrow$ only pole from $M_j(z;t)^{-1}$
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