DEEP LEARNING AND FREE PROBABILITY: TRAINING AND GENERALIZATION DYNAMICS IN HIGH DIMENSIONS

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OUTLINE

- 1. Motivation / Introduction
- 2. Case Study: Linear Regression
- 3. Linearization pt 1: High-Dimensional Kernels
- 4. Linearization pt 2: The Linear Pencil
- 5. Linearization pt 3: Neural Tangent Kernel

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DATASETS ARE OFTEN HIGH-DIMENSIONAL

Many common datasets have both a large number of samples and a large number of features

- CIFAR-10 (10⁵ samples, 10⁴ features)
- Imagenet (10⁷ samples, 10⁵ features)

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Many modalities are intrinsically high-dimensional:

- Speech (high frequency, large dynamic range)
- Video (high frame rates, high resolution)
- DNA sequences (large number of base pairs)

DEEP LEARNING MODELS ARE HIGH-DIMENSIONAL

Deep learning models employ large numbers of parameters. At least two practically-relevant high-dimensional regimes:

- 1. Linearly overparameterized ($p \sim m$)
- 2. Quadratically overparameterized $(n_l \sim m)$

Examples:

	Width n_l	# Samples <i>M</i>	# Parameters p
FC/ CIFAR-10	10 ³	104	106
ResNet/ ImageNet	10 ³	107	108

HIGH-DIMENSIONAL SCALING LIMITS

We will focus on the following high-dimensional asymptotics of zero and one hidden-layer networks:

- 1. Dataset size $m \to \infty$
- 2. Input dimensionality $n_0 \to \infty$
- 3. Hidden-layer size $n_1 \to \infty$

with the ratios
$$\phi = \frac{n_0}{m}$$
 and $\psi = \frac{n_0}{n_1}$ held constant

MARCHENKO-PASTUR DISTRIBUTION

In the low-dimensional (standard) regime, certain statistics may be simple:

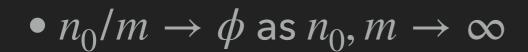
- Dataset $X \in \mathbb{R}^{n_0 \times m}$, $X_{ij} \sim \mathcal{N}(0,1)$
- For n_0 finite, infinite samples ($m \to \infty$), $\frac{1}{m}XX^T \to I_{n_0}$

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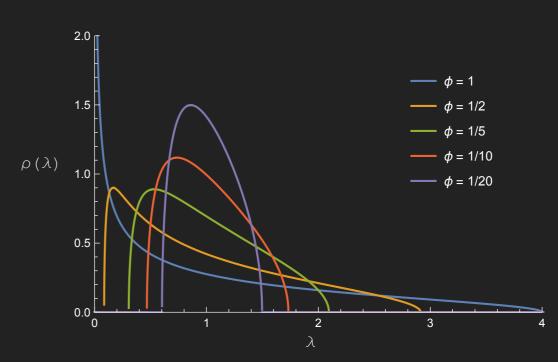
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In the high-dimensional regime, spectrum can be non-trivial



$$\bullet \ \rho(\frac{1}{m}XX^T) \to MP(\phi)$$



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LINEAR REGRESSION

Consider one of the simplest possible learning problems, linear ridge regression with iid Gaussian inputs and targets.

$$L = \|WX - Y\|_F^2 + \gamma \|W\|_F^2$$
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$$W^* = YQX^T, \qquad Q = (X^TX + \gamma I)^{-1}$$

$$E_{train} = ||W^*X - Y||_F^2 = tr[(YQX^TX - Y)^T(YQX^TX - Y)]$$

$$= tr[X^TXQY^TYQX^TX] - 2tr[X^TXQY^TY] + tr[Y^TY]$$

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RESOLVENT AND STIELTJES TRANSFORM

The training error depends on the trace of the resolvent Q

$$E_{train} = -\gamma^2 \partial_{\gamma} tr[Q] \qquad Q = (X^T X + \gamma I)^{-1}$$

This trace tr[Q] is known as the Cauchy transform $G: \mathbb{C}^+ \to \mathbb{C}^+$,

$$G(z) = -tr[(X^T X - zI)^{-1}] = \int \frac{1}{z - \lambda} \rho_{X^T X}(\lambda) d\lambda$$

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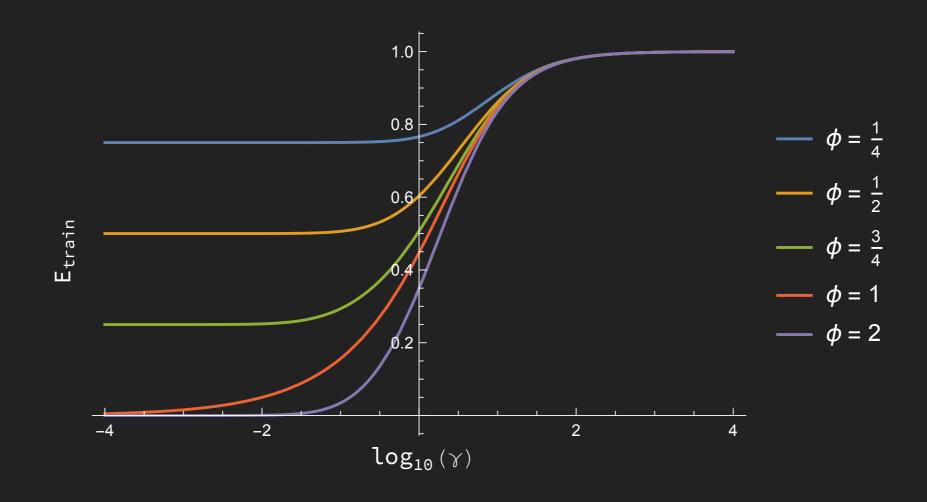
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$$= \frac{1 - (1 - z)\phi + \sqrt{(1 - (1 - z)\phi)^{2} - 4z\phi}}{2z} \qquad \phi = \frac{n_{0}}{m}$$

HIGH-DIMENSIONAL TRAINING ERROR

$$E_{train} = \frac{\sqrt{(\gamma\phi + \phi - 1)^2 + 4\gamma\phi}(\phi(\gamma\phi + \gamma + \phi - 2) + 1)}{2\phi(\gamma((\gamma + 2)\phi + 2) + \phi - 2) + 2} + \frac{1 - \phi}{2} \qquad \phi = \frac{n_0}{m}$$



GRADIENT DESCENT

Let's optimize the regression weights using gradient descent.

$$L = \|WX - Y\|_F^2 + \gamma \|W\|_F^2, \qquad X_{ij} \sim \mathcal{N}(0,1), \ Y_{ij} \sim \mathcal{N}(0,1)$$

$$W(t) = YQ(t)X^T \qquad Q(t) = K^{-1}(I - (I - 2\eta K)^t)$$

 $K = X^T X + \gamma I$

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Now the training error has a simple time-dependent expression:

$$\begin{split} E_{train}(t) &= tr[X^T X Q(t)^2 X^T X] - 2tr[X^T X Q(t)] + 1 \\ &= tr[(K - \gamma I)^2 Q(t)^2] - 2tr[(K - \gamma I) Q(t)] + 1 \\ &= tr[K^{-2}((K - \gamma I)(I - 2\eta K)^t + \gamma I)] \end{split}$$

TIME-DEPENDENCE THROUGH CAUCHY'S FORMULA

$$E_{train}(t) = tr[f(K)]$$
 $f(K) = K^{-2}((K - \gamma I)(I - 2\eta K)^t + \gamma I)^2$

Recalling Cauchy's integral formula for matrix functions,

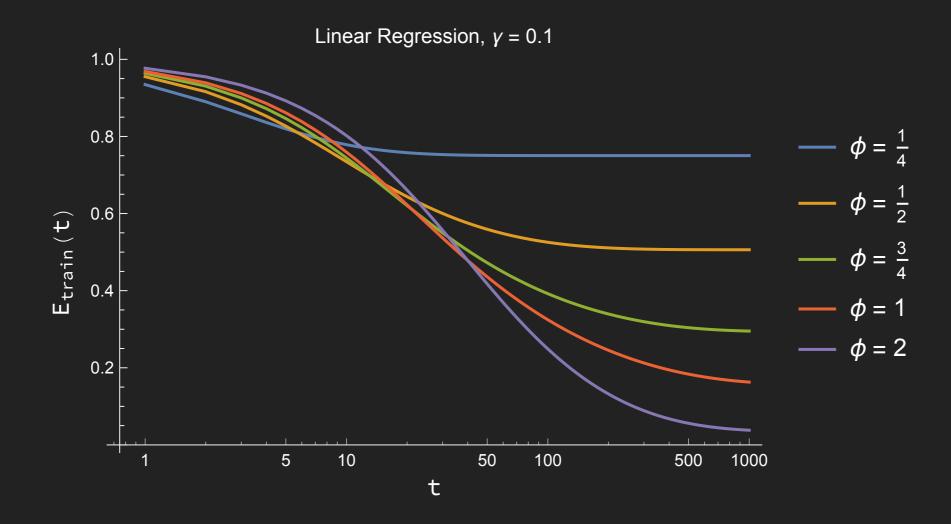
$$f(A) = \frac{1}{2\pi i} \int_C f(z)(A - zI)^{-1} dz$$

Taking the trace of this equation gives,

$$E_{train}(t) = \frac{1}{2\pi i} \int_{C} \frac{((z - \gamma)(1 - 2\eta z)^{t} + \gamma)^{2}}{z^{2}} G(z - \gamma) dz$$

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Consider random nonlinear features $F = f(W_1X)$

$$L = \|WF - Y\|_F^2 + \gamma \|W\|_F^2, \qquad X_{ij}, Y_{ij}, [W_1]_{ij} \sim \mathcal{N}(0,1)$$

$$W(t) = YQ(t)F^{T}$$

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Identical to linear regression, but $X^TX \to F^TF$

$$E_{train}(t) = \frac{1}{2\pi i} \int_{C} \frac{((z - \gamma)(1 - 2\eta z)^{t} + \gamma)^{2}}{z^{2}} G(z - \gamma) dz$$

$$G(z) = -tr[(F^T F - zI)^{-1}] = \int \frac{1}{z - \lambda} \rho_{F^T F}(\lambda) d\lambda$$

1. Naive option: method of moments

$$G(z) = tr[(zI - F^T F)^{-1}] = \frac{1}{n_1} \sum_{k} \frac{1}{z^{k+1}} \mathbb{E} tr[(F^T F)^k]$$

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$$\mathbb{E} \frac{1}{n_1} tr[(F^T F)^k] = \frac{1}{n_1} \frac{1}{m^k} \mathbb{E} \left[\sum_{i_1, \dots, i_k \in [n_1]} F_{i_1 \mu_1} F_{i_2 \mu_1} F_{i_2 \mu_2} F_{i_3 \mu_2} \cdots F_{i_k \mu_k} F_{i_1 \mu_k} \right]_{\mu_1, \dots, \mu_k \in [m]}$$

Can be evaluated to leading order

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$$F \simeq F^{lin} \equiv \sqrt{\zeta} WX + \sqrt{\eta - \zeta} A$$

$$\eta = \int dz \, \frac{e^{-z^2/2}}{\sqrt{2\pi}} f(\sigma_w \sigma_x z)^2 \qquad \qquad \zeta = \left[\sigma_w \sigma_x \int dz \, \frac{e^{-z^2/2}}{\sqrt{2\pi}} f'(\sigma_w \sigma_x z) \right]^2 \qquad \qquad A_{ij} \sim \mathcal{N}(0,1)$$

- 2. Better option: "strong universality" + free probability
 - ii) Free probability algebraic formalism that allows adding and multiplying "freely independent" noncommutative random variables

If A, W, X are free then the Cauchy transform of F can be obtained from the Cauchy transforms of A, W, X.

$$F \simeq F^{lin} \equiv \sqrt{\zeta} WX + \sqrt{\eta - \zeta} A$$

$$\{G_X, G_W\} \rightarrow S_{WX} \rightarrow G_{WX} \rightarrow R_{WX}$$

$$G_A \rightarrow R_A$$
 $R_{WX+A} \rightarrow G_{F^TF}$

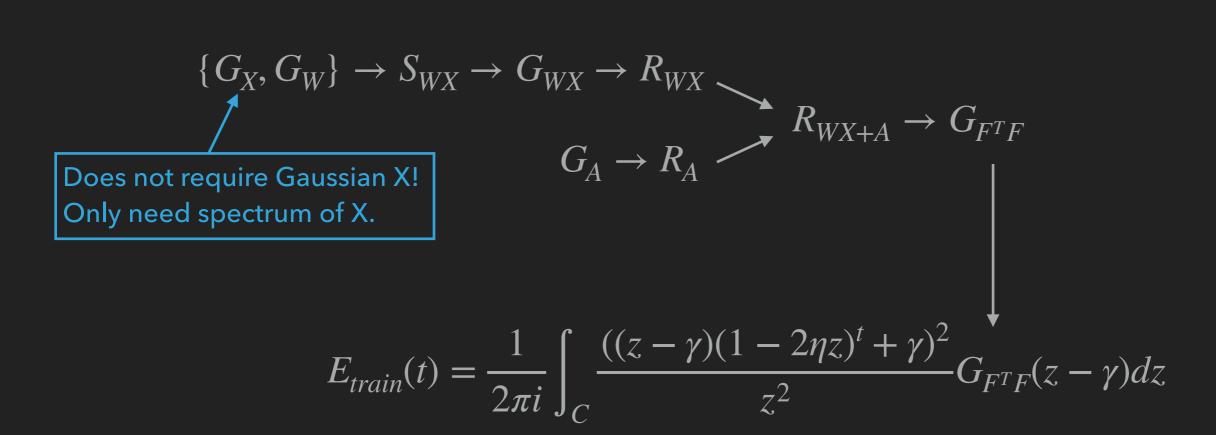
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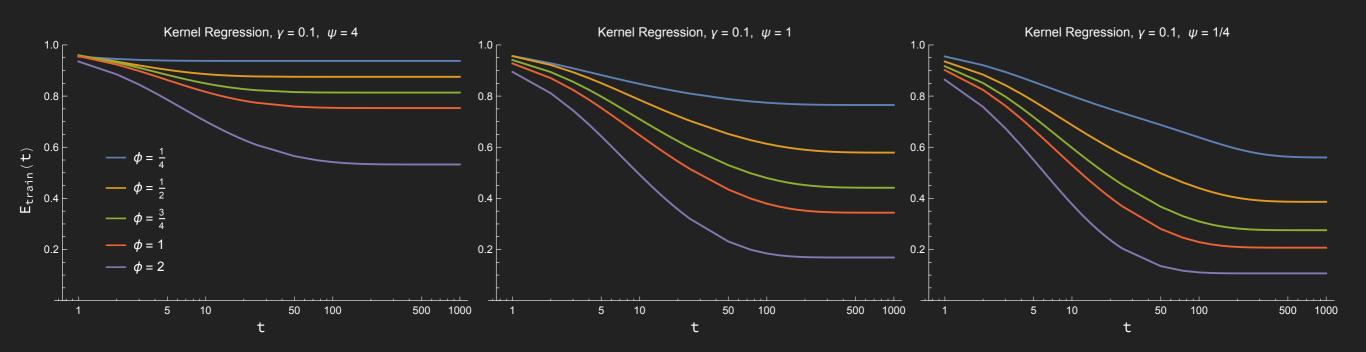
$$R_{WX+A} \rightarrow G_{F^TF}$$

$$\downarrow$$

$$E_{train}(t) = \frac{1}{2\pi i} \int_C \frac{((z-\gamma)(1-2\eta z)^t + \gamma)^2}{z^2} G_{F^TF}(z-\gamma) dz$$



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$$\phi = \frac{n_0}{m} \qquad \qquad \psi = \frac{n}{n}$$

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GENERALIZATION ERROR

To discuss generalization, need a non-trivial model for the joint (X, Y) distribution.

For concreteness, consider the student-teacher setup, where $Y=V_2g(V_1X)$ for fixed, random weights.

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For concreteness, consider the student-teacher setup, where $Y = V_2 g(V_1 X)$ for fixed, random weights.

As we saw for F, in high dimensions Y can also be replaced with a linearized version having the correct second moments,

$$Y \simeq Y^{lin} \equiv \sqrt{\zeta_g} V_2 V_1 X + \sqrt{\eta_g - \zeta_g} V_2 B \qquad B_{ij} \sim \mathcal{N}(0,1)$$

$$\eta_g = \int dz \, \frac{e^{-z^2/2}}{\sqrt{2\pi}} g(\sigma_w \sigma_x z)^2 \qquad \zeta_g = \left[\sigma_w \sigma_x \int dz \, \frac{e^{-z^2/2}}{\sqrt{2\pi}} g'(\sigma_w \sigma_x z) \right]^2$$

$$L = \|WF - Y\|_F^2 + \gamma \|W\|_F^2, \qquad Y = V_2 g(V_1 X) \qquad F = f(W_1 X)$$

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Consider an unseen test point \tilde{x} , with random features $\tilde{f} = f(W_1 \tilde{x})$ and targets $\tilde{y} = V_2 g(V_1 \tilde{x})$.

$$E_{test} = \mathbb{E}_{\tilde{x}} \|W^* \tilde{f} - \tilde{y}\|_F^2 = \mathbb{E}_{\tilde{x}} tr[(YQF^T \tilde{f} - \tilde{y})^T (YQF^T \tilde{f} - \tilde{y})]$$

$$= \mathbb{E}_{\tilde{x}} tr[\tilde{f}^T F Q Y^T Y Q F^T \tilde{f}] - 2\mathbb{E}_{\tilde{x}} tr[\tilde{f}^T F Q Y^T \tilde{y}] + \mathbb{E}_{\tilde{x}} tr[\tilde{y}^T \tilde{y}]$$

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Now, utilize "strong universality" to apply the linearization,

$$Y \to Y^{lin} \equiv \sqrt{\zeta_g} V_2 V_1 X + \sqrt{\eta_g - \zeta_g} V_2 B \qquad F \to F^{lin} \equiv \sqrt{\zeta} W_1 X + \sqrt{\eta - \zeta} A$$
$$\tilde{y} \to \tilde{y}^{lin} \equiv \sqrt{\zeta_g} V_2 V_1 \tilde{x} + \sqrt{\eta_g - \zeta_g} V_2 \tilde{b} \qquad \tilde{f} \to \tilde{f}^{lin} \equiv \sqrt{\zeta} W_1 \tilde{x} + \sqrt{\eta - \zeta} \tilde{a}$$

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After applying the linearization,

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The expectations over $V_1, V_2, B, \tilde{b}, \tilde{a}$ are trivial because

$$Q \to ((F^{lin})^T F^{lin} + \gamma I)^{-1} = \left((\sqrt{\zeta} W_1 X + \sqrt{\eta - \zeta} A)^T (\sqrt{\zeta} W_1 X + \sqrt{\eta - \zeta} A) \right)^{-1}$$

depends only on W_1, X, A .

After applying linearization and performing the trivial expectations, the result can be written as

$$E_{test} = \sum_{i} tr[R_{i}QS_{i}Q] + \sum_{i} tr[T_{i}Q]$$

where R_i , S_i , T_i are low-order polynomials in W_1 , X, A.

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Q: How to evaluate the trace of a *rational function* of random matrices?

A: Linearization + operator-valued free probability

RATIONAL FUNCTIONS AS BLOCK MATRIX OPERATIONS

Any rational function of non-commutative variables can be represented in terms of the inverse of a matrix whose entries are linear in the variables.

$$R(x_1, ..., x_k) = u^T M^{-1} v$$
, $M = M_0 + \sum_i M_i x_i$

This representation is called the linear pencil.

Constructive proof by induction: manifestly true for k=1, and higher k follow if the representation is closed under addition, multiplication, and inversion. These follow from Schur complement formula.

EXAMPLE OF LINEAR PENCIL

Consider the resolvent as a function in W, X, A,

$$Q = ((F^{lin})^T F^{lin} - zI)^{-1} = ((WX + A)^T (WX + A) - zI)^{-1}$$

$$= u^T M^{-1} v = (I \quad 0 \quad 0 \quad 0) \begin{pmatrix} -zI & A^T & X^T & 0 \\ -A & I & 0 & -W \\ 0 & -W^T & I & 0 \\ -X & 0 & 0 & I \end{pmatrix}^{-1} \begin{pmatrix} I \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

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M is linear in the W, X, A:

$$M = \begin{pmatrix} -zI & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{pmatrix} + \begin{pmatrix} 0 & 0 & X^T & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -X & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -W \\ 0 & -W^T & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & A^T & 0 & 0 \\ -A & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

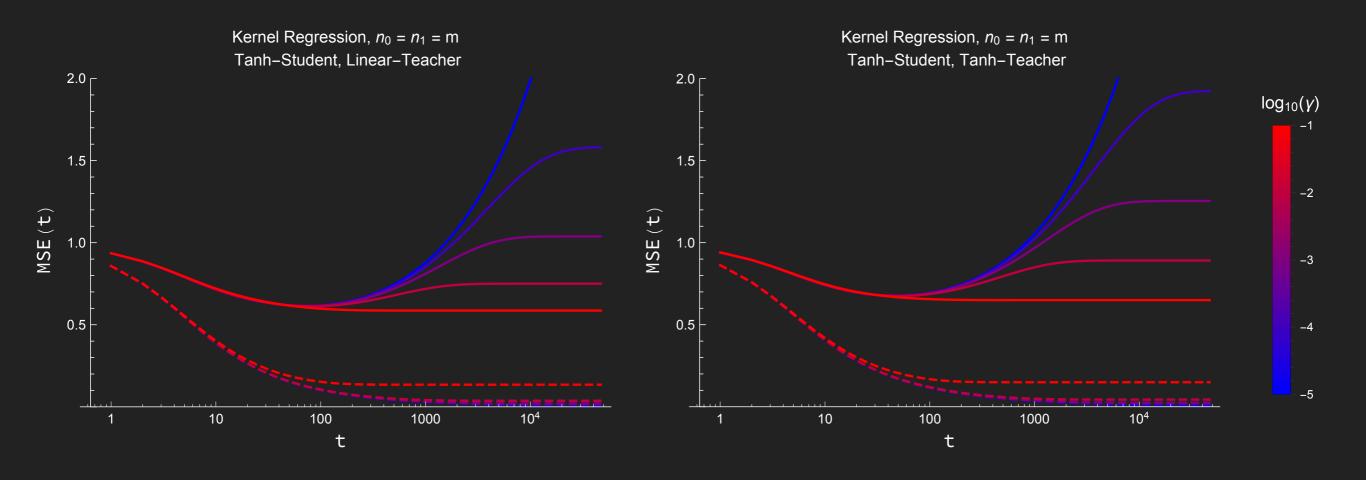
but the additive terms are not free, owing to the block structure.

EXAMPLE OF LINEAR PENCIL

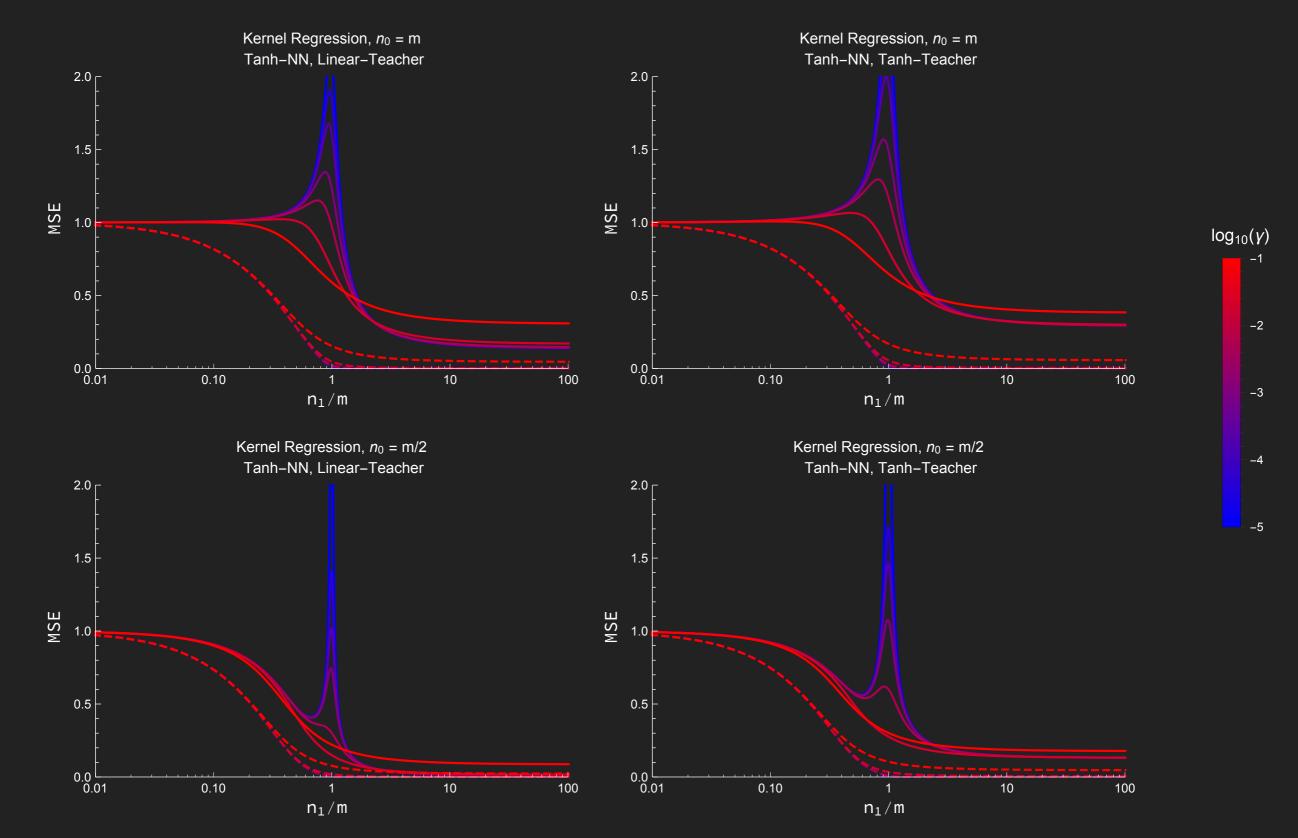
However, we can view M as a linear function of the W, X, A with coefficients in $M_4(\mathbb{C})$

and then freeness can be salvaged, but one must account for the non-commutativity of the coefficients in $M_4(\mathbb{C})$

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This motivates a linear approximation

$$N(x; \theta(t)) \approx N(x; \theta(0)) + \frac{\partial N}{\partial \theta} \Big|_{\theta = \theta(0)} (\theta(t) - \theta(0)) + \mathcal{O}(\theta(t) - \theta(0))^2$$

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The dynamics are determined by the Neural Tangent Kernel

$$\Theta = J_0^T J_0 = \Theta_1 + \Theta_2 = (F')^T D_{W_2} F' \odot X^T X + F^T F \qquad F' = f'(W_1 X)$$

NEURAL TANGENT KERNEL

The offset N_0 contributes unnecessary variance. Can set $N_0=0$ by subtracting two copies of the model with same initialization

$$\begin{split} N^{VR}(x; \{\theta_1, \theta_2\}) &= \frac{1}{\sqrt{2}} \big(N(x; \theta_1) - N(x; \theta_2) \big) \\ N_0^{VR} &= 0, \quad \Theta^{VR} = \Theta \end{split}$$

NEURAL TANGENT KERNEL: SECOND-LAYER KERNEL

The component of the kernel from the second layer is the same random features kernel studied before, $\Theta_2 = K = F^T F$

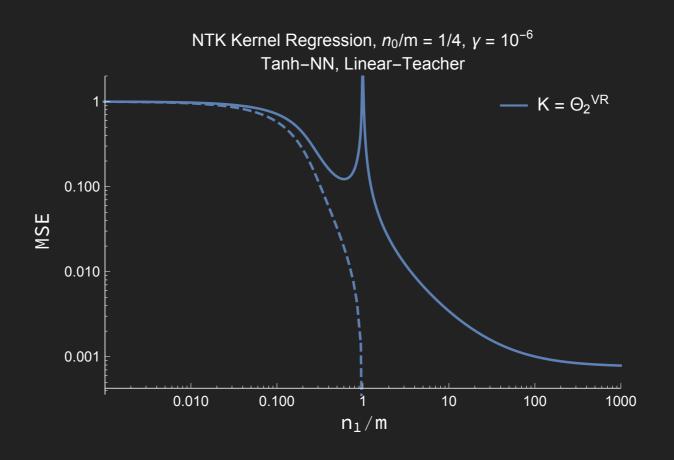
It has non-trivial random matrix behavior in the high-dimensional limit when $n_0 \sim n_1 \sim m$

NEURAL TANGENT KERNEL: FIRST-LAYER KERNEL

The first layer kernel has a Hadamard product structure, $\Theta_1 = (F')^T D_{W_2} F' \odot X^T X$. It has two non-trivial scaling regimes:

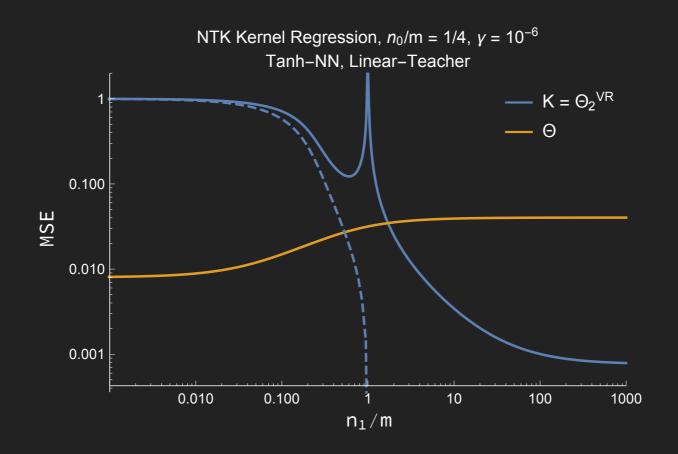
- 1. Linearly overparameterized $(n_0 n_1 \sim m)$
 - Fluctations of $(F')^T D_{W_2} F'$ are important
 - n eigenvalues of $\mathcal{O}(n)$ and n^2 of $\mathcal{O}(1)$
- 2. Quadratically overparameterized ($n_l \sim m$)
 - Only the mean of $(F')^T D_{W_2} F'$ is important
 - $\bullet \ \ \Theta_1 \simeq \Theta_1^{lin} = c_1 \overline{I + c_2 X^T X}$

QUADRATIC OVERPARAMETERIZATION



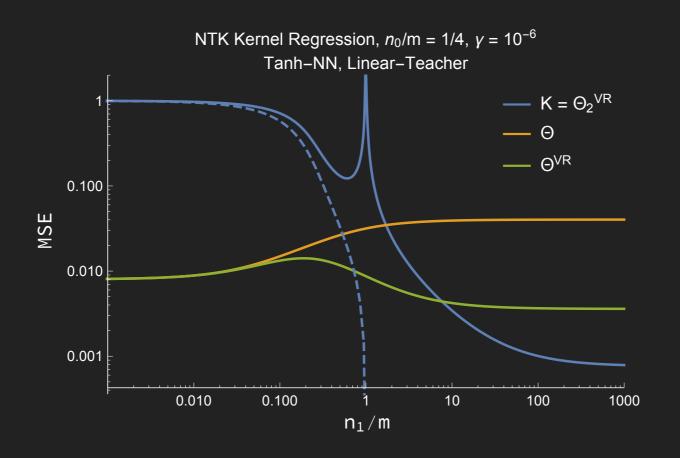
QUADRATIC OVERPARAMETERIZATION

The network can be too overparametrized

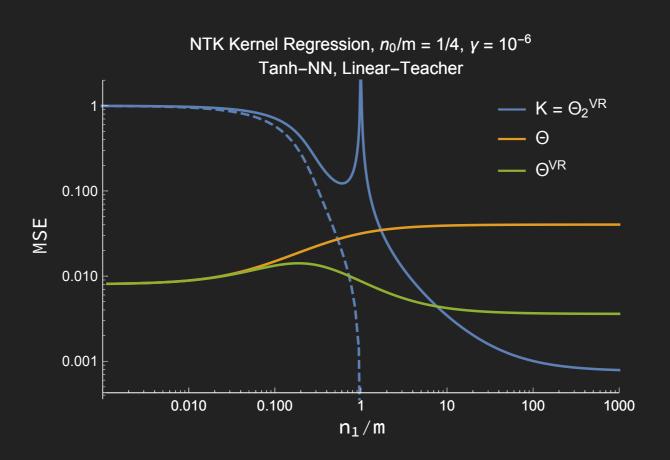


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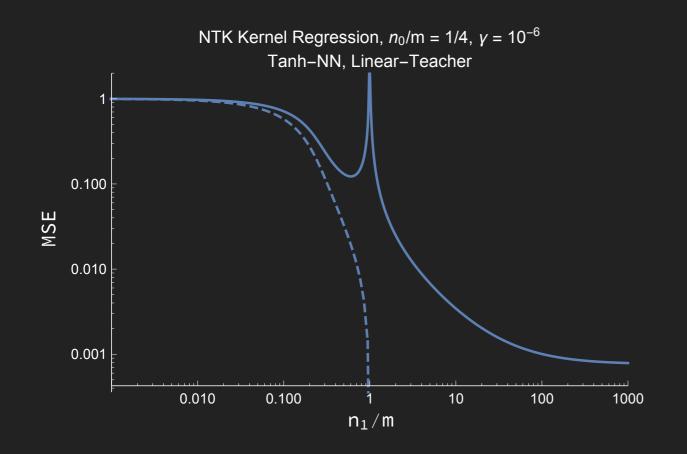
Reducing the variance helps, but a peak emerges

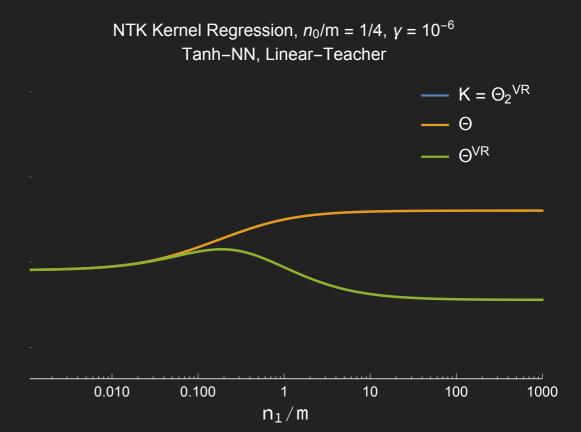


TWO OVERPARAMETERIZATION SCALES

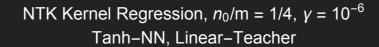


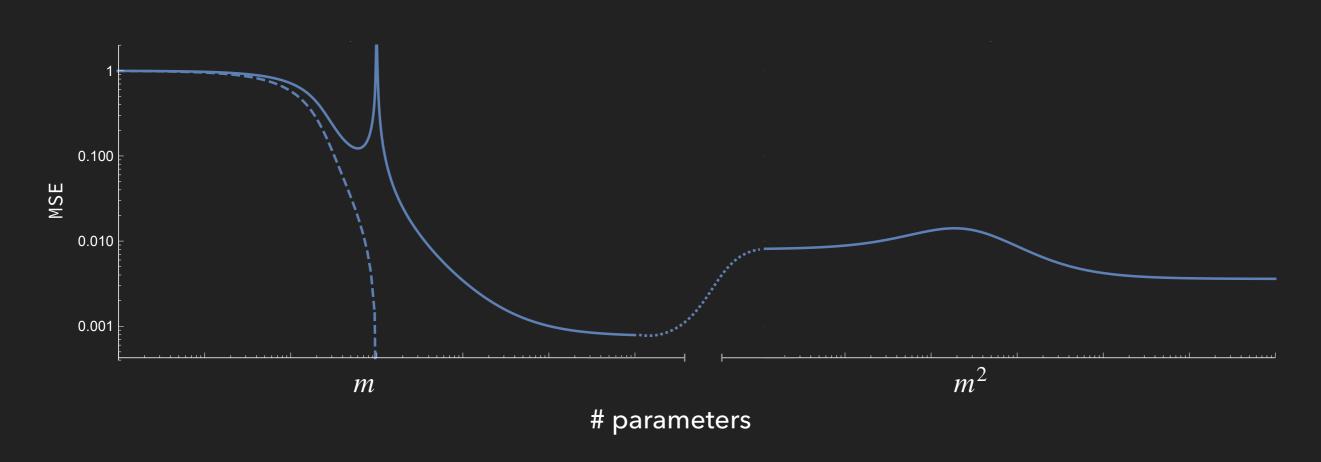
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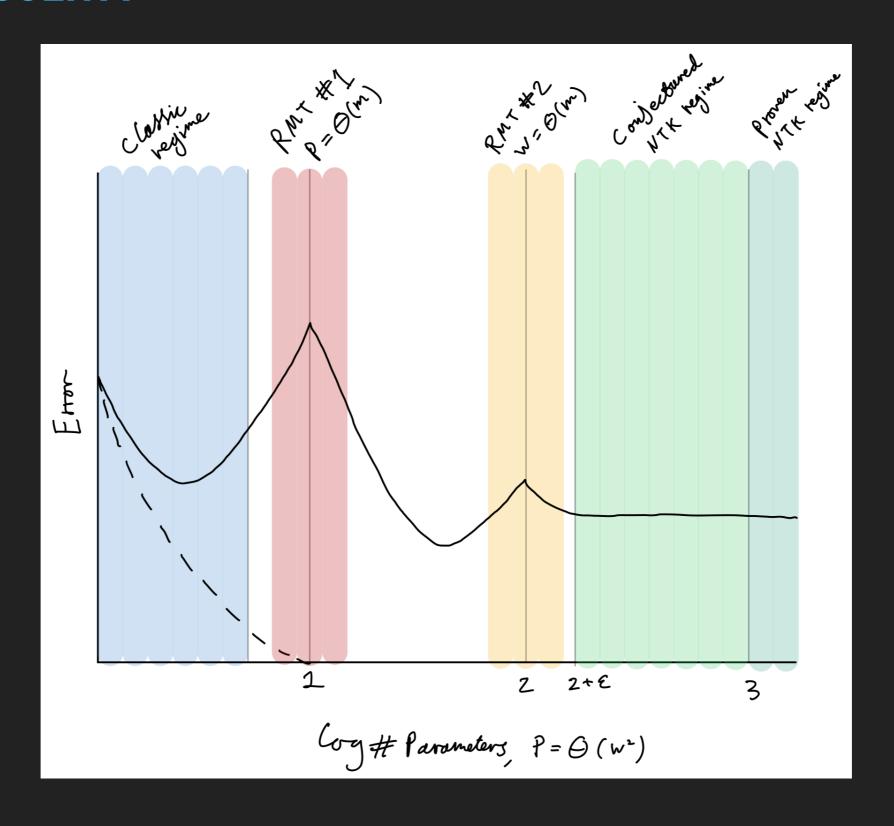


TWO OVERPARAMETERIZATION SCALES





TRIPLE DESCENT?



EXTRA SLIDES

CUMULANTS AND CLASSICAL INDEPENDENCE

The cumulant generating function K generates connected correlation functions via the relation

$$K(t_1, ..., t_n) = \log \mathbb{E} e^{\sum_{i=1}^n t_i X_i}$$

The cumulants κ are defined by the moments via a sum over partitions π :

$$\mathbb{E}[X_1 \cdots X_n] = \sum_{\pi} \kappa_{\pi}[X_1, \dots, X_n] \qquad \kappa_{\pi}[X_1, \dots, X_n] = \prod_{B \in \pi} \kappa[X_i : i \in B]$$

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For example,

n=1:
$$\mathbb{E}[X_1] = \kappa[X_1]$$

n=2:
$$\mathbb{E}[X_1X_2] = \kappa[X_1X_2] + \kappa[X_1]\kappa[X_2]$$

CUMULANTS AND CLASSICAL INDEPENDENCE

n=3:
$$\mathbb{E}[X_1X_2X_3] = \kappa[X_1X_2X_3] + \kappa[X_1X_2]\kappa[X_3] + \kappa[X_1X_3]\kappa[X_2] + \kappa[X_2X_3]\kappa[X_1] + \kappa[X_1X_2]\kappa[X_3] + \kappa[X_1X_2]\kappa[X_3]$$

The mixed cumulants vanish for independent random variables

FREE CUMULANTS AND FREE INDEPENDENCE

Free cumulants: sum over non-crossing partitions $\pi \in NC(n)$:

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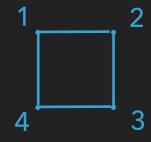
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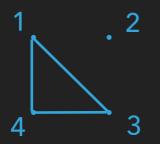
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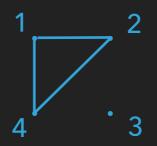
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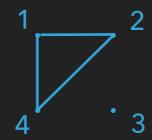












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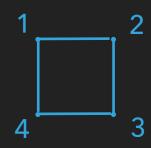
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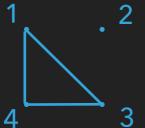












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$$\text{n=4:} \quad \mathbb{E}[X_{1}X_{2}X_{3}X_{4}] = \kappa[X_{1}X_{2}X_{3}X_{4}] + \kappa[X_{1}X_{2}X_{3}]\kappa[X_{4}] + \kappa[X_{1}X_{2}X_{4}]\kappa[X_{3}] \\ + \kappa[X_{1}X_{3}X_{4}]\kappa[X_{2}] + \kappa[X_{2}X_{3}X_{4}]\kappa[X_{1}] + \kappa[X_{1}X_{2}]\kappa[X_{3}X_{4}] \\ + \kappa[X_{1}X_{3}]\kappa[X_{2}X_{4}] + \kappa[X_{1}X_{4}]\kappa[X_{2}X_{3}] + \kappa[X_{3}X_{4}]\kappa[X_{1}]\kappa[X_{2}] \\ + \kappa[X_{2}X_{4}]\kappa[X_{1}]\kappa[X_{3}] + \kappa[X_{2}X_{3}]\kappa[X_{1}]\kappa[X_{4}] + \kappa[X_{1}X_{4}]\kappa[X_{2}]\kappa[X_{3}] \\ + \kappa[X_{1}X_{3}]\kappa[X_{2}]\kappa[X_{4}] + \kappa[X_{1}X_{2}]\kappa[X_{3}]\kappa[X_{4}] + \kappa[X_{1}]\kappa[X_{2}]\kappa[X_{3}]$$

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S-transform: G(z) = S(zG(z) - 1)(z(G(z) - 1))

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$$S_{A}S_{B} = S_{AB} \rightarrow G_{AB}(z) \rightarrow \rho_{AB}(\lambda)$$

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