Applications of random matrix theory to graph matching and neural networks

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In this talk, I’ll discuss applications of random matrix theory to two (unrelated) problems in statistics and machine learning:

- Graph matching
- Spectral analysis of neural network kernel matrices
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- Graph matching
- Spectral analysis of neural network kernel matrices

I’ll focus on high-level ideas, discuss the random matrix connections, and describe a few open questions.
Graph Matching
Graph matching

Joint work with:

Cheng Mao  Yihong Wu  Jiaming Xu
Given the LinkedIn network, can you de-anonymize Twitter? More abstractly: Given two correlated random graphs on $n$ vertices, with a hidden correspondence between their vertices, can you recover this vertex matching?
Given the LinkedIn network, can you de-anonymize Twitter?

[Picture courtesy of R. Srikant]
Given the LinkedIn network, can you de-anonymize Twitter?

More abstractly: Given two *correlated* random graphs on $n$ vertices, with a hidden correspondence between their vertices, can you recover this vertex matching?
Correlated Erdős-Rényi graph model

\[ A_{ij}, B_{ij} \sim \text{Bernoulli}(q) \quad \text{and} \quad \mathbb{P}[A_{ij} = B_{ij} = 1] = (1 - \delta)q \]
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\( q \) is the sparsity, and \( \delta \) is the fraction of differing edges. Different edge pairs \((i, j)\) are independent. [Pedarsani, Grossglauser '11]
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q \text{ is the sparsity, and } \delta \text{ is the fraction of differing edges.} \\
\text{Different edge pairs } (i, j) \text{ are independent. } [\text{Pedarsani, Grossglauser '11}] \\
\text{We observe } A \text{ and } \Pi_*^T B \Pi_* \text{ and want to recover } \Pi_*.
\end{align*}
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We observe \( A \) and \( \Pi^* B \Pi_* \) and want to recover \( \Pi_* \). Questions:

- How correlated must \( A \) and \( B \) be, to recover \( \Pi_* \) w.h.p.?
- How to design a computational algorithm that achieves this?
Spectral algorithms

Use the (permutation invariant) eigendecompositions

\[ A = \sum_{i=1}^{n} \lambda_i u_i u_i^\top \quad \text{and} \quad B = \sum_{j=1}^{n} \mu_j v_j v_j^\top \]
Spectral algorithms

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- **Top eigenvector**: Match \( A \) to \( B \) by sorting \( u_1 \) and \( v_1 \). Similar ideas in IsoRank [Singh, Xu, Berger ’08], EigenAlign [Feizi et al ’19].
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\[
\sum_{i=1}^{n} v_i^\top \Pi u_i \equiv \text{Tr } X \Pi \quad \text{where} \quad X = \sum_{i=1}^{n} u_i v_i^\top
\]

This aligns every \( u_i \) with the corresponding \( v_i \). [Umeyama ’88]
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Both work in noiseless settings (\( \delta = 0 \)), but are brittle to noise: Each pair \((u_i, v_i)\) decorrelates when \( \delta > 1/n^\alpha \) for some \( \alpha > 0 \).
A new spectral algorithm: GRAMPA

GRAph Matching by Pairwise eigen-Alignments

1. Compute the eigendecompositions

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2. Construct the similarity matrix

\[ X = \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \mu_j)^2 + \eta^2} \times \underbrace{u_i u_i^\top J v_j v_j^\top}_{\text{“Alignment” between } u_i \text{ and } v_j} \]

where \( \eta \) = bandwidth parameter, \( J \) = all-1’s matrix.
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where \( \eta = \) bandwidth parameter, \( J = \) all-1’s matrix.

3. Find the permutation \( \Pi \) which maximizes \( \text{Tr} \, X \Pi \). This tries to align every \( u_i \) with every \( v_j \), with weighting by the Cauchy kernel.
Motivation for GRAMPA

Isomorphic Erdős-Rényi graphs (500 vertices, edge probability $\frac{1}{2}$)

$\langle u_{100}, v_j \rangle^2$ for $j \in \{80, \ldots, 120\}$, averaged across 1000 simulations
Motivation for GRAMPA

Erdős-Rényi graphs with fraction of differing edges $\delta = 0.001$

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Erdős-Rényi graphs with fraction of differing edges $\delta = 0.05$

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Cauchy kernel applied to \( \lambda_i \) and \( \mu_j \)
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“Alignment” between \( u_i \) and \( v_j \)

The Cauchy kernel may be motivated by eigenvector correlation decay in the Dyson Brownian motion model

\[ B = A + Z_\delta \]

where \( Z \overset{\text{d}}{=} \sqrt{\delta} \times \text{independent GOE} \). Results of [Benigni '17] show, using analysis of the eigenvector moment flow in [Bourgade, Yau '17], that

\[ n \cdot E[\langle u_i, v_j \rangle^2] \approx \frac{\delta}{(\lambda_i - \mu_j)^2 + C\delta^2} \]
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\[ X = \sum_{i,j=1}^{n} \frac{\eta}{(\lambda_i - \mu_j)^2 + \eta^2} \times \left\{ \begin{array}{c} u_i u_i^\top J v_j v_j^\top \end{array} \right\} \]

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\[ n \cdot \mathbb{E}[\langle u_i, v_j \rangle^2] \approx \frac{\delta}{(\lambda_i - \mu_j)^2 + C\delta^2} \]

[Question: Is this true also for a time-evolving Erdős-Rényi model?]
Theorem (F., Mao, Wu, Xu)

For the correlated Erdős-Rényi model with edge probability $q \geq \text{polylog}(n)/n$ and fraction of differing edges $\delta \leq 1/\text{polylog}(n)$, this algorithm recovers the true vertex correspondence $\Pi^*$ w.h.p.
Theoretical guarantee

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- Improves over previous spectral algorithms requiring $\delta \leq 1/n^{\alpha}$.
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- This is currently the best-known guarantee for polynomial-time algorithms. Matches previous result of [Ding, Ma, Wu, Xu '18].
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- [Barak, Chou, Lei, Schramm, Sheng '18] developed an $n^{O(\log n)}$-time algorithm, which succeeds for $\delta \leq 1 - \varepsilon$ and $q \geq n^\varepsilon/n$.
- [Ganassali, Massoulié '20] developed a polynomial-time algorithm that recovers a positive fraction of the vertex matchings, for $\delta \leq 1 - c$ and $q \asymp 1/n$. 
Main ideas of the analysis

Define the resolvents

\[ R_A(z) = (A - z \text{Id})^{-1} \quad R_B(z) = (B - z \text{Id})^{-1} \]

**Lemma**

*The GRAMPA similarity matrix \( X \) has the resolvent representation*

\[
X = \frac{1}{2\pi} \text{Re} \oint_{\Gamma} R_A(z)JR_B(z + i\eta)dz
\]

This contour \( \Gamma \) contains all of the poles of \( R_A \), and none of the poles of \( R_B \).
Main ideas of the analysis

Suppose $\Pi^* = \text{Id}$, and consider the $(k, \ell)$ entry

$$X_{k\ell} = \frac{1}{2\pi} \text{Re} \oint_{\Gamma} \left[ e_k^T R_A(z) J R_B(z + i\eta) e_\ell \right] dz$$
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$$X_{k\ell} = \frac{1}{2\pi} \text{Re} \int_{\Gamma} \left[ e_k^\top R_A(z)JR_B(z + i\eta)e_\ell \right] dz$$

**Diagonal:** By Schur-complement identities,

$$X_{kk} \approx \frac{1}{2\pi} \text{Re} a_k^\top \left[ \int_{\Gamma} m(z)m(z + i\eta)R_{A(k)}(z)JR_{B(k)}(z + i\eta) dz \right] b_k$$

$(a_k, b_k)$ in $(A, B)$ are correlated, and independent of $(A^{(k)}, B^{(k)})$. 
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$(a_k, b_k)$ in $(A, B)$ are correlated, and independent of $(A^{(k)}, B^{(k)})$.

**Off-diagonal:** Similarly,

$$X_{k\ell} \approx \frac{1}{2\pi} \text{Re} a_k^\top \left[ \oint_{\Gamma} m(z)m(z + i\eta) R_{A(k\ell)}(z) J R_{B(k\ell)}(z + i\eta) \right] b_\ell$$

$(a_k, b_\ell)$ are independent, and also independent of $(A^{(k\ell)}, B^{(k\ell)})$. 
Main ideas of the analysis

Applying local law estimates and fluctuation averaging techniques from [Erdős, Knowles, Yau, Yin ’13], we analyze the traces and Frobenius norms of the preceding integrals.
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When $\Pi^* = \text{Id}$,

$$\min_k X_{kk} > \max_{k \neq \ell} X_{k\ell} \quad \text{w.h.p.}$$

Then the permutation $\Pi$ maximizing $\text{Tr } X\Pi$ is $\Pi = \text{Id}$, so GRAMPA returns $\text{Id}$ w.h.p.

By permutation invariance of the algorithm, GRAMPA returns $\Pi^*$ w.h.p. for any true permutation $\Pi^*$. 
A different motivation for GRAMPA

\[
\min_{\Pi \in S_n} \| A - \Pi^\top B \Pi \|_F^2 = \min_{\Pi \in S_n} \| \Pi A - B \Pi \|_F^2
\]
A different motivation for GRAMPA

\[ \min_{\Pi \in S_n} \| A - \Pi^\top B \Pi \|_F^2 = \min_{\Pi \in S_n} \| \Pi A - B \Pi \|_F^2 \]

Relax this to the quadratic program

\[ \min_{X \in \text{conv}(S_n)} \| XA - BX \|_F^2 \]

for the convex hull \( \text{conv}(S_n) = \{X : X_{ij} \geq 0, X1 = 1, X^\top 1 = 1\} \).
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Solve this for \( X \), then round to a permutation \( \Pi \).

[Zaslavskiy, Bach, Vert ’09], [Aflalo, Bronstein, Kimmel ’15]
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[Zaslavskiy, Bach, Vert ’09], [Aflalo, Bronstein, Kimmel ’15]

This method is not well-understood for the Erdős-Rényi model. The GRAMPA matrix \( X \) is, instead, the further relaxation

\[
\min_{X : 1^T X1 = n} \| XA - BX \|_F^2 + \eta^2 \| X \|_F^2
\]
A hierarchy of relaxations

Full QP: \( \min_{X \in \text{conv}(S_n)} \| XA - BX \|_F^2 \)

- \( \min_{X: \vec{x}_1 = 1, \vec{x}^T \vec{1} = 1} \| XA - BX \|_F^2 \)
- \( \min_{X: \|X\|_F = 1} \| XA - BX \|_F^2 \)
- \( \min_{X: \|X\|_F = 1} \| XA - BX \|_F^2 + \eta^2 \|X\|_F^2 \)
- \( \min_{X: \vec{1}^T X = n} \| XA - BX \|_F^2 + \eta^2 \|X\|_F^2 \)

GRAMPA: \( \min_{X: \vec{1}^T X = n} \| XA - BX \|_F^2 + \eta^2 \|X\|_F^2 \)
A hierarchy of relaxations

These two relaxations have representations in terms of the spectra of $A$ and $B$, and we analyze them in our work.
A hierarchy of relaxations

Full QP: \[
\min_{X \in \text{conv}(S_n)} \|XA - BX\|_F^2
\]

\[
\min_{X: X_1=1, X^T 1 = 1} \|XA - BX\|_F^2
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\[
\min_{X: X_1=1} \|XA - BX\|_F^2 + \eta^2 \|X\|_F^2
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GRAMPA: \[
\min_{X: 1^T X_1 = n} \|XA - BX\|_F^2 + \eta^2 \|X\|_F^2
\]

\[
\min_{X: x_{ij} \geq 0, \|X\|_F^2 = 1} \|XA - BX\|_F^2
\]

Variants of this are related to the resolvent-type matrix

\[
\left[ (A \otimes \text{Id} - \text{Id} \otimes B)^2 + \eta^2 (J \otimes \text{Id} + \text{Id} \otimes J) \right]^{-1}
\]

for the Kronecker model \( A \otimes \text{Id} - \text{Id} \otimes B \in \mathbb{R}^{n^2 \times n^2}. \)
A hierarchy of relaxations

How to analyze these programs with entrywise non-negativity is open. We believe from simulation that these may achieve exact recovery of $\Pi^*$ w.h.p. up to $\delta \leq c$ for some constant $c > 0$. 
Neural network kernel matrices
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Joint work with Zhichao Wang:
Feedforward neural network

Function $f_\theta : \mathbb{R}^{d_0} \to \mathbb{R}, \ x \mapsto f_\theta(x)$, defined iteratively by

$x^1 = \sigma(W_1x), \ x^2 = \sigma(W_2x^1), \ldots, \ x^L = \sigma(W_Lx^{L-1}), \ f_\theta(x) = w^\top x^L$

$\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function, applied entrywise.

Two fundamental questions:

• How does learning occur during gradient descent training of $\theta$?

• What allows $f_\theta(x)$ to generalize to unseen test samples?
Feedforward neural network

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$\mathbf{x}^1 = \sigma(\mathbf{W}_1 \mathbf{x})$, $\mathbf{x}^2 = \sigma(\mathbf{W}_2 \mathbf{x}^1)$, $\ldots$, $\mathbf{x}^L = \sigma(\mathbf{W}_L \mathbf{x}^{L-1})$, $f_\theta(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}^L$

- $\mathbf{W}_1 \in \mathbb{R}^{d_1 \times d_0}$, $\mathbf{W}_2 \in \mathbb{R}^{d_2 \times d_1}$, $\ldots$, $\mathbf{W}_L \in \mathbb{R}^{d_L \times d_{L-1}}$, and $\mathbf{w} \in \mathbb{R}^{d_L}$ are the weights. We denote $\theta = (\mathbf{W}_1, \ldots, \mathbf{W}_L, \mathbf{w})$.
- $\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function, applied entrywise.
Feedforward neural network

Function $f_\theta : \mathbb{R}^{d_0} \to \mathbb{R}$, $x \mapsto f_\theta(x)$, defined iteratively by

\[ x^1 = \sigma(W_1 x), \quad x^2 = \sigma(W_2 x^1), \ldots, \quad x^L = \sigma(W_L x^{L-1}), \quad f_\theta(x) = w^\top x^L \]

- $W_1 \in \mathbb{R}^{d_1 \times d_0}$, $W_2 \in \mathbb{R}^{d_2 \times d_1}$, $\ldots$, $W_L \in \mathbb{R}^{d_L \times d_{L-1}}$, and $w \in \mathbb{R}^{d_L}$ are the weights. We denote $\theta = (W_1, \ldots, W_L, w)$.
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- How does learning occur during gradient descent training of $\theta$?
- What allows $f_\theta$ to generalize to unseen test samples?
Two kernel matrices

Let \( X = (x_1, \ldots, x_n) \in \mathbb{R}^{d_0 \times n} \) be the training samples, and \( X_\ell \in \mathbb{R}^{d_\ell \times n} \) the outputs of each layer \( \ell = 1, \ldots, L \).

Recent theory of neural networks highlights two kernel matrices:

1. The **Conjugate Kernel** (or equivalent Gaussian process kernel)
   \[
   K_{\text{CK}} = X_L^\top X_L \in \mathbb{R}^{n \times n}
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The final step of the network is just linear regression on \( X_L \). \( K^{\text{CK}} \) governs the properties of this linear regression.
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The final step of the network is just linear regression on $X_L$. $K_{\text{CK}}$ governs the properties of this linear regression.

- The network is often already predictive when $X_L$ is fixed by random initialization of $W_1, \ldots, W_L$, and only $w$ is trained.
- For $d_1, \ldots, d_L \to \infty$ and fixed $n$, $K_{\text{CK}}$ converges to a limit kernel, and this is an approximation of regression in an associated RKHS.

[Neal ’94], [Williams ’97], [Cho, Saul ’09], [Rahimi, Recht ’09], [Daniely et al ’16], [Poole et al ’16], [Schoenholz et al ’17], [Lee et al ’18], ...
2. The **Neural Tangent Kernel**

\[
K^{\text{NTK}} = (\nabla_\theta f_\theta(X))^\top (\nabla_\theta f_\theta(X)) \in \mathbb{R}^{n \times n}
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Two kernel matrices

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Training errors evolve during gradient descent as

\[ \frac{d}{dt} \left( y - f_\theta(t)(X) \right) = -K^{\text{NTK}}(t) \cdot \left( y - f_\theta(t)(X) \right) \]
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- For \( d_1, \ldots, d_L \to \infty \) and fixed \( n \), \( K^{\text{NTK}} \) is constant over training.
- Then (diagonalizing \( K^{\text{NTK}} \)) \( y - f_{\theta(t)}(X) \to 0 \) at a different exponential rate along each eigenvector of \( K^{\text{NTK}} \).

[Jacot, Gabriel, Hongler ’19], [Du et al ’19], [Allen-Zhu et al ’19], [Lee et al ’19], ...
Two kernel matrices

2. The **Neural Tangent Kernel**

\[ K^{\text{NTK}} = (\nabla_\theta f_\theta(X))^\top (\nabla_\theta f_\theta(X)) \in \mathbb{R}^{n \times n} \]

Training errors evolve during gradient descent as

\[
\frac{d}{dt} \left( y - f_\theta(t)(X) \right) = -K^{\text{NTK}}(t) \cdot \left( y - f_\theta(t)(X) \right)
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Infinitely wide neural nets are equivalent to kernel linear regression.
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Infinitely wide neural nets are equivalent to kernel linear regression. Neural nets of practical width often generalize better than these equivalent kernel models. [Chizat et al '18], [Arora et al '19]
Eigenvalues in the linear width regime

We study the eigenvalue distributions of $K_{CK}$ and $K_{NTK}$

- In a *linear width* regime where $n/d_\ell \to \gamma_\ell \in (0, \infty)$ for each $\ell$

Theorem (F., Wang)
For fixed $L$, almost surely as $n, d_1, \ldots, d_L \to \infty$,

$$\lim \text{spec} K_{CK} = \mu_{CK}, \quad \lim \text{spec} K_{NTK} = \mu_{NTK}$$

for two probability distributions $\mu_{CK}$ and $\mu_{NTK}$. These are defined by $\mu_0$ and properties of $\sigma(x)$. 
Eigenvalues in the linear width regime

We study the eigenvalue distributions of $K^C$ and $K^{NT}$

- In a *linear width* regime where $n/d_\ell \to \gamma_\ell \in (0, \infty)$ for each $\ell$
- At random (i.i.d. Gaussian) initialization of the weights $\theta$
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- Assuming that the training samples $X = (x_1, \ldots, x_n)$ are approximately pairwise orthogonal, and $\lim \text{spec} X^\top X = \mu_0$

(I’ll use “lim spec” to denote weak convergence of the e.s.d.)
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Approximate pairwise orthogonality

Normalizing training samples such that \( \|x_1\|^2, \ldots, \|x_n\|^2 \approx 1 \), we require

\[
|x_\alpha^\top x_\beta| \leq \varepsilon_n
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for each pair \( \alpha \neq \beta \in \{1, \ldots, n\} \), where \( \varepsilon_n \ll n^{-1/4} \).
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This holds with $\varepsilon_n \approx 1/\sqrt{n}$ if $d_0 \approx n$ and $x_1, \ldots, x_n$ are mean-zero independent samples with some concentration. For example:

- $x_\alpha = z_\alpha$ where $z_\alpha$ has i.i.d. subgaussian entries
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- $x_\alpha = \Sigma^{1/2} z_\alpha$ where $\|\Sigma\|$ is bounded
- $x_\alpha = f(z_\alpha)$ where entries of $z_\alpha$ satisfy a log-Sobolev inequality, and $f$ is any Lipschitz function
Limit spectral distribution of the CK

Let

$$\mu \mapsto \rho^\text{MP}_\gamma \boxtimes \mu$$

be the Marcenko-Pastur map for the spectra of sample covariance matrices with aspect ratio $\gamma$.

Theorem (F., Wang)

For each $\ell = 1, \ldots, L$,

$$\lim \text{spec} X_\ell^T X_\ell = \mu_\ell.$$ 

So

$$\lim \text{spec} K_{\text{CK}} = \mu_L.$$ 

• For one layer, this is closely related to existing results of [Pennington, Worah '17], [Louart, Liao, Couillet '18].

• When $b\sigma = 0$, each $\mu_\ell = \rho^\text{MP}_\gamma$ is a Marcenko-Pastur law. This case was shown (for $X$ with i.i.d. entries) by [Benigni, Péché '19].

We normalize $\sigma$ so that $E[\sigma(\xi)] = 0$, $E[\sigma(\xi)^2] = 1$. 

\[1\]
Limit spectral distribution of the CK

Let
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be the Marcenko-Pastur map for the spectra of sample covariance matrices with aspect ratio \( \gamma \). For \( \ell = 1, \ldots, L \), define
\[ \mu_{\ell} = \rho_{\gamma_{\ell}}^{\text{MP}} \boxtimes \left( (1 - b_{\sigma}^2) + b_{\sigma}^2 \cdot \mu_{\ell-1} \right) \]
where \( b_{\sigma} = \mathbb{E}_{\xi \sim \mathcal{N}(0,1)}[\sigma'(\xi)] \).\(^1\)

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**Theorem (F., Wang)**

*For each $\ell = 1, \ldots, L$, $\lim \text{spec } X_\ell^\top X_\ell = \mu_\ell$. So $\lim \text{spec } K^{\text{CK}} = \mu_L$.*

---

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\(^1\)We normalize \( \sigma \) so that \( \mathbb{E}[\sigma(\xi)] = 0, \mathbb{E}[\sigma(\xi)^2] = 1. \)
Lemma

There are constants $q_{-1}, \ldots, q_L$ defined by $\sigma(x)$, such that

$$\lim \text{spec } K^{NTK} = \lim \text{spec } \left( q_{-1} \text{Id} + \sum_{\ell=0}^{L} q_{\ell} X_{\ell}^\top X_{\ell} \right)$$
Limit spectral distribution of the NTK

**Lemma**

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**Theorem (F., Wang)**

Consider any $z = (z_{-1}, \ldots, z_L), w = (w_{-1}, \ldots, w_L)$. Then

$$\frac{1}{n} \text{Tr} \left( z_{-1} \text{Id} + \sum_{\ell=0}^{L} z_{\ell} X^{\top}_{\ell} X_{\ell} \right)^{-1} \left( w_{-1} \text{Id} + \sum_{\ell=0}^{L} w_{\ell} X^{\top}_{\ell} X_{\ell} \right)$$

has a deterministic limit $t_L(z, w)$. A fixed-point equation defines each function $t_{\ell}$ in terms of $t_{\ell-1}$. 
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has a deterministic limit $t_L(z, w)$. A fixed-point equation defines each function $t_{\ell}$ in terms of $t_{\ell-1}$. The limit Stieltjes transform for $K^{NTK}$ is then

$$m(z) = t_L \left( (-z + q_{-1}, q_0, \ldots, q_L), (1, 0, \ldots, 0) \right).$$
Simulations for i.i.d. Gaussian $X$

Simulated eigenvalues in blue, limit spectral distribution in red

$\sigma(x) \propto \tan^{-1}(x)$, $L = 5$, $n = 3000$, $d_0 = 1000$, $d_1 = \ldots = d_5 = 6000$
Simulations for input images from CIFAR-10

5000 random training images from CIFAR-10, w/ top 10 PCs removed to improve pairwise orthogonality

$$\sigma(x) \propto \tan^{-1}(x),\ L = 5,\ n = 5000,\ d_0 = 3072,\ d_1 = \ldots = d_5 = 10000$$
Main ideas of the analysis

Lemma

Suppose the input data $X$ is $\varepsilon_n$-orthogonal. Then each $X_1, \ldots, X_L$ is $C\varepsilon_n$-orthogonal for a constant $C \equiv C(L) > 0$, w.h.p.

This allows us to induct on the layer $\ell$, and analyze each matrix $X_\ell^T X_\ell$ conditional on $X_0, \ldots, X_{\ell-1}$. 
Main ideas of the analysis

Recall $X_\ell = \sigma(W_\ell X_{\ell-1})$, and observe that

- $X_\ell$ has i.i.d. rows with law $\sigma(w^T X_{\ell-1})$, conditional on $X_{\ell-1}$
Main ideas of the analysis

Recall $X_\ell = \sigma(W_\ell X_{\ell-1})$, and observe that

- $X_\ell$ has i.i.d. rows with law $\sigma(w^T X_{\ell-1})$, conditional on $X_{\ell-1}$
- Consequently, $\lim \text{spec } X_\ell^T X_\ell$ is the Marcenko-Pastur map of

$$\Phi_\ell = \mathbb{E}_w[\sigma(w^T X_{\ell-1}) \otimes \sigma(w^T X_{\ell-1})]$$

[Louart, Liao, Couillet '18]
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  \Phi_\ell = \mathbb{E}_w[\sigma(w^T X_{\ell-1}) \otimes \sigma(w^T X_{\ell-1})]
  \]
  [Louart, Liao, Couillet '18]

When $X_{\ell-1}$ is $\varepsilon_n$-orthogonal, we show that

\[
\frac{1}{n} \left\| \Phi_\ell - \left( (1 - b_\sigma^2) \text{Id} + b_\sigma^2 X_{\ell-1}^T X_{\ell-1} \right) \right\|_F^2 \lesssim n \cdot \varepsilon_n^4 \to 0.
\]

So $\lim \text{spec } \Phi_\ell = (1 - b_\sigma^2) + b_\sigma^2 \mu_{\ell-1}$. 
Main ideas of the analysis

To analyze $K^{\text{NTK}}$, we characterize inductively the limit $t_\ell(z, w)$ of

$$\frac{1}{n} \text{Tr} \left( z_{-1} \text{Id} + \sum_{k=0}^{\ell} z_k X_k^\top X_k \right)^{-1} \left( w_{-1} \text{Id} + \sum_{k=0}^{\ell} w_k X_k^\top X_k \right)$$
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Remove $X_\ell^\top X_\ell$ from the numerator, by writing this as

$$\frac{w_\ell}{z_\ell} + \frac{1}{n} \text{Tr} \left( A + z_\ell X_\ell^\top X_\ell \right)^{-1} M$$

where $A, M$ are linear combinations of $X_0^\top X_0, \ldots, X_{\ell-1}^\top X_{\ell-1}, \text{Id}$. 
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where $A, M$ are linear combinations of $X_0^\top X_0, \ldots, X_{\ell-1}^\top X_{\ell-1}, \operatorname{Id}$.

Conditional on $X_0, \ldots, X_{\ell-1}$, these matrices $A$ and $M$ are deterministic, and $X_\ell$ is random with i.i.d. rows having second-moment matrix $\Phi_\ell$. 
Main ideas of the analysis

We show an approximation

$$\frac{1}{n} \text{Tr} \left( A + z_\ell X_\ell^\top X_\ell \right)^{-1} M \approx \frac{1}{n} \text{Tr} \left( A + s_\ell^{-1} \Phi_\ell \right)^{-1} M$$

where $s_\ell$ approximately satisfies the fixed-point equation

$$s_\ell \approx \frac{1}{z_\ell} + \frac{\gamma_\ell}{n} \text{Tr} \left( A + s_\ell^{-1} \Phi_\ell \right)^{-1} \Phi_\ell.$$

This equation depends on the joint spectral limit of $(A, \Phi_\ell)$. 
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This equation depends on the joint spectral limit of \((A, \Phi_\ell)\). Applying \( \Phi_\ell \approx (1 - b_\sigma^2) \text{Id} + b_\sigma^2 X_{\ell-1}^\top X_{\ell-1} \) and the induction hypothesis for \( \ell - 1 \), this has a limit in terms of \( t_{\ell-1}(z, w) \).

We show inductively that the limit equation has a unique fixed point \( s_\ell \in \mathbb{C}^+ \). This then defines \( t_\ell \) recursively in terms of \( t_{\ell-1} \), by

\[
t_\ell(z, w) = \lim_{n \to \infty} \frac{1}{n} \text{Tr} \left( A + s_\ell^{-1} \Phi_\ell \right)^{-1} M
\]
Propagation of “signal” at random initialization

Consider a spiked input matrix

\[ X = s_1 u_1 v_1^T + s_2 u_2 v_2^T + \text{i.i.d. Gaussian noise} \]
Propagation of “signal” at random initialization

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X = s_1 u_1 v_1^\top + s_2 u_2 v_2^\top + \text{i.i.d. Gaussian noise}
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Eigenvalues of \(X^\top X\), for \(u_1, u_2, v_1, v_2\) uniform on the sphere
Propagation of “signal” at random initialization

Eigenvalues of $X_\ell^\top X_\ell$, when $v_1, v_2$ are each supported on 20 samples
Propagation of “signal” at random initialization

Eigenvalues of $X_\ell^\top X_\ell$, when $v_1, v_2$ are each supported on 20 samples

Question: Can we understand the propagation of outlier eigenvalues and eigenvectors through these layers?

Related analysis of Gaussian mixture models for one hidden layer, and other kernels: [Couillet, Benaych-Georges ’16], [Liao, Couillet ’18]
Evolution of spectra over training

Eigenvalues of $K^{\text{CK}}$ and $K^{\text{NTK}}$ for a trained 3-layer network

$L = 3, n = 1000, d_0 = 800, d_1 = d_2 = d_3 = 800$
Evolution of spectra over training

Eigenvalues of $K^{CK}$ and $K^{NTK}$ for a trained 3-layer network

$L = 3, n = 1000, d_0 = 800, d_1 = d_2 = d_3 = 800$

Trained on $(x_\alpha, y_\alpha)$ pairs where $x_\alpha$ are uniform on the sphere, and

$$y_\alpha = \sigma(v^\top x_\alpha)$$

Final prediction-$R^2$ of the trained model was 0.81. The spectral bulks elongate, and large outliers emerge over training.
Outliers contain information about training labels.

Projection of training labels $\mathbf{y}$ onto top 2 PC’s of the trained $K^{\text{CK}}$ explains 96% of the variance. The emergence of these outliers is the main mechanism of training in this example.
Outliers contain information about training labels

Projection of training labels $\mathbf{y}$ onto top 2 PC’s of the trained $K^{CK}$ explains 96% of the variance. The emergence of these outliers is the main mechanism of training in this example.

Question: Can we understand the evolutions of $K^{CK}$ and/or $K^{NTK}$ over training, from a spectral perspective?

Related work on the evolution of the NTK in an entrywise size: [Huang, Yau ’19], [Dyer, Gur-Ari ’19]
References

Graph matching:


Neural network kernel matrices: