Recent Developments in Nonlinear Random Matrices

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Nonlinear random matrix: an entry-wise nonlinear function applied to a given random matrix

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- Kernel matrix K, $K(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_i, \mathbf{x}_j)$. e.g., $K_{ij} = f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle)$, $f(||\mathbf{x}_i \mathbf{x}_j||)$. Kernel PCA, kernel SVM, kernel regression.
- Kernel matrices from neural networks.
- Random graphs from nonlinear random matrices.

Random inner product matrix, proportional regime

- Random data $x_1, \ldots, x_n \in \mathbb{R}^d$, mean zero, variance 1. $d/n \to \gamma$.
- Random inner product kernel matrix

$$\boldsymbol{K}_{ij} = \begin{cases} \frac{1}{\sqrt{d}} f\left(\frac{1}{\sqrt{d}} \langle \boldsymbol{x}_i, \boldsymbol{x}_j \rangle\right) & i \neq j \\ 0 & i = j. \end{cases}$$

- x_i Gaussian [Cheng-Singer 13], universality [Do-Vu 13].
- $a = \mathbb{E}_{\xi \sim N(0,1)}[\xi f(\xi)], \quad \nu = \mathbb{E}[f(\xi)^2], \quad \mathbb{E}[f(\xi)] = 0.$

• Limiting spectral distribution of K:

$$a(\mu_{\mathrm{MP},\gamma}-1)\boxplus\sqrt{\gamma^{-1}(
u-a^2)}\mu_{sc}.$$

• f(x) = x, $\nu = a^2$, Marchenko-Pastur law.

• a = 0, semicircle.

Concentration

[Fan-Montanari 19] Hermite expansion of f(x):

$$f(x) = \sum_{i=1}^{\infty} a_i h_i(x),$$

 $h_i(x)$ normalized hermite polynomials. Decomposition

$$oldsymbol{\mathcal{K}} = \sum_{i=1}^\infty \mathsf{a}_i oldsymbol{\mathcal{K}}_i.$$

 $a_1 \mathbf{K}_1$ has a Marchenko-Pastur law, $\sum_{i\geq 2}^{\infty} a_i \mathbf{K}_i$ has a semicircle law.

- *x_i* Gaussian, *f* is odd, *f*(*x*) = −*f*(*x*). ||*K*|| converges to the edge of the limiting spectrum.
- Non-asymptotic bound on ||*K*||.
- General distribution \mathbf{x}_i , possible outliers depending on $\mathbb{E}[\mathbf{x}_{ij}^4]$ and a_2 .

A different scaling, proportional regime

$$\boldsymbol{K}_{ij} = f\left(rac{1}{d}\langle \boldsymbol{x}_i, \boldsymbol{x}_j
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Theorem (Operator norm approximation, El Karoui 10)

Let $\Sigma = \mathbb{E} \mathbf{x} \mathbf{x}^{\top}$. Assume $\mathbf{z} = \Sigma^{-1/2} \mathbf{x}$ has independent entries with zero mean and unit variance, where $\mathbb{E} |z_i|^{4+\eta} \leq M$, $\|\Sigma\| \leq M$, $\frac{\operatorname{Tr} \Sigma}{d} \to \tau$. With high probability, when $n, d \to \infty$ proportionally,

$$\left\| \boldsymbol{K} - c_0 \mathbf{1} \mathbf{1}^\top - c_1 \frac{\boldsymbol{X} \boldsymbol{X}^\top}{d} - c_2 \mathbf{I}_n \right\| = o(1), \quad \text{where}$$

 $c_0 = f(0) + \frac{f''(0)}{2} \frac{\operatorname{Tr}(\Sigma^2)}{d^2}, \quad c_1 = f'(0), \quad c_2 = f\left(\frac{\operatorname{Tr}(\Sigma)}{d}\right) - f(0) - f'(0) \frac{\operatorname{Tr}(\Sigma)}{d}.$

 \implies Marchenko-Pastur law for **K**.

[El Karoui 10]: Taylor expansion

$$\mathbf{K}_{ij} = f\left(\frac{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}{d}\right).$$

When $n \simeq d$,

• **Off-diagonal**: $\frac{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}{d} \approx 0$. Taylor expansion at 0,

$$f\left(\frac{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}{d}\right) \approx f(0) + f'(0) \frac{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}{d} + \frac{f''(0)}{2} \left(\frac{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}{d}\right)^2 + \frac{f'''(\zeta_{ij})}{6} \left(\frac{\langle \mathbf{x}_i, \mathbf{x}_j \rangle}{d}\right)^3$$

• **Diagonal**: $\frac{\langle \mathbf{x}_i, \mathbf{x}_i \rangle}{d} \approx \frac{\operatorname{tr} \boldsymbol{\Sigma}}{d} \approx \tau$. Taylor expansion at τ ,

$$f\left(\frac{\langle \mathbf{x}_i, \mathbf{x}_i \rangle}{d}\right) pprox f(\tau) + f'(\zeta_{ii})\left(\frac{\langle \mathbf{x}_i, \mathbf{x}_i \rangle}{d} - \tau\right).$$

• Control error terms: $\|\boldsymbol{K} - c_0 \mathbf{1} \mathbf{1}^\top + c_1 \frac{\mathbf{X} \mathbf{X}^\top}{d} + c_2 \mathbf{I}_n\| = o(1).$

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- K has a "low-rank+ bulk + regularizer" structure.

Fully-connected neural network

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

$$f_{\theta}(\mathbf{x}) = \mathbf{w}^{\top} \frac{1}{\sqrt{d_L}} \sigma \bigg(\mathbf{W}_L \frac{1}{\sqrt{d_{L-1}}} \sigma \bigg(\dots \frac{1}{\sqrt{d_2}} \sigma \bigg(\mathbf{W}_2 \frac{1}{\sqrt{d_1}} \sigma (\mathbf{W}_1 \mathbf{x}) \bigg) \bigg) \bigg).$$



- $W_1 \in \mathbb{R}^{d_1 \times d_0}$, $W_2 \in \mathbb{R}^{d_2 \times d_1}$, ..., $W_L \in \mathbb{R}^{d_L \times d_{L-1}}$, and $\mathbf{w} \in \mathbb{R}^{d_L}$. Training parameters: $\theta = (W_1, \ldots, W_L, \mathbf{w})$.
- Training samples in a matrix: $X_0 = (\mathbf{x}_1, \dots, \mathbf{x}_n) \in \mathbb{R}^{d_0 \times n}$.
- σ : activation function, e.g. $\frac{e^{\alpha x}}{1+e^{\alpha x}}$ (Sigmoid), |x|, max(0, x) (ReLU).

•
$$\boldsymbol{X}_{\ell} = \frac{1}{\sqrt{d_{\ell}}} \sigma \left(\boldsymbol{W}_{\ell} \boldsymbol{X}_{\ell-1} \right) \in \mathbb{R}^{d_{\ell} \times n}$$
, for $1 \leq \ell \leq L$.

Conjugate kernel

$$\pmb{K}_\ell^{\mathsf{CK}} = \pmb{X}_\ell^{ op} \pmb{X}_\ell \in \mathbb{R}^{n imes n}$$

- *K*^{CK}_ℓ governs the properties of random feature regression or network with only the output layer trained.
- At random initialization, its limiting spectrum was studied when all d_i/d_{i-1} and d₀/n are proportional. [Pennington-Worah 17], [Benigni-Péché 19], [Louart-Liao-Couillet 18], [Fan-Wang 20]

Spectrum of conjugate kernels: deterministic data

$$L = 1, \quad \mathbf{Y} = \frac{1}{N} \sigma(\mathbf{W}\mathbf{X})^{\top} \sigma(\mathbf{W}\mathbf{X}),$$

 $\boldsymbol{W} \in \mathbb{R}^{N \times d}, \boldsymbol{X} \in \mathbb{R}^{d \times n}. \ N/d \to \alpha_1, n/d \to \alpha_2, \ N/n \to \gamma.$

- Deterministic data X, W Gaussian, Lipschitz activation σ. Row vectors of σ(WX) are independent. [Louart-Liao-Couillet 18]
- Limiting spectral distribution of Y is μ_{MP} ⊠ μ_Φ, where μ_Φ is the limiting spectral distribution of

$$\boldsymbol{\Phi} = \mathbb{E}_{\boldsymbol{W}}[\boldsymbol{Y}] = \mathbb{E}_{\boldsymbol{w}}[\sigma(\boldsymbol{w}^{\top}\boldsymbol{X})^{\top}\sigma(\boldsymbol{w}^{\top}\boldsymbol{X})] \in \mathbb{R}^{n \times n}.$$

- Same limiting ESD as a linear model $\frac{1}{N} \mathbf{P}^{\top} \mathbf{W}^{\top} \mathbf{W} \mathbf{P}$ with $\mathbf{P}^{\top} \mathbf{P} = \Phi$, $\mathbf{P} \in \mathbb{R}^{d \times n}$.
- Key step: concentration of random quadratic forms σ(w^TX)A σ(w^TX)^T for deterministic A.

• When columns of X are approximately orthonormal [Fang-Wang 20],

$$\mu = \rho_{\gamma}^{\mathsf{MP}} \boxtimes \left((1 - b_{\sigma}^2) + b_{\sigma}^2 \cdot \mu_{\mathbf{X}^{\top} \mathbf{X}} \right),$$

where $b_{\sigma} = \mathbb{E}_{\xi \sim \mathbb{N}(0,1)}[\sigma'(\xi)], \quad \mathbb{E}[\sigma(\xi)] = 0, \ \mathbb{E}[\sigma(\xi)^2] = 1.$

• From [LLC 18] and a first order approximation $\Phi \approx (1 - b_{\sigma}^2) \mathbf{I} + b_{\sigma}^2 \mathbf{X} \mathbf{X}^{\top}$.

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- Can be extended to *L* layers. Approximate orthogonality propagates through the nonlinear map *X*_{ℓ-1} → *X*_ℓ = ¹/_{√dℓ} σ(*WX*_{ℓ-1}).

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- Can be extended to *L* layers. Approximate orthogonality propagates through the nonlinear map $X_{\ell-1} \to X_{\ell} = \frac{1}{\sqrt{d_{\ell}}} \sigma(WX_{\ell-1})$.
- L = 1, N ≫ n, deformed semicircle law for Y [Wang-Z. 24]. Training and generalization error with deterministic data [Wang-Z. 23, Latourelle-Vigeant Paquette 23].

Spectrum of conjugate kernels: random data

- Universality [Benigni-Péché 19], i.i.d. entries in X, W with mean zero, variance 1, general distributions, σ analytic.
- The limiting spectral distribution depends on

$$\theta_1(\sigma) = \mathbb{E}_{\xi \sim N(0,1)}[\sigma^2(\xi)], \qquad \theta_2(\sigma) = \left(\mathbb{E}_{\xi \sim N(0,1)}[\sigma'(\xi)]\right)^2.$$

• Same as the limiting ESD of an information-plus-noise matrix:

$$\boldsymbol{M} = \frac{1}{N} \left(\frac{\sqrt{\theta_2}}{\sqrt{d}} \boldsymbol{W} \boldsymbol{X} + \sqrt{\theta_1 - \theta_2} \boldsymbol{Z} \right) \left(\frac{\sqrt{\theta_2}}{\sqrt{d}} \boldsymbol{W} \boldsymbol{X} + \sqrt{\theta_1 - \theta_2} \boldsymbol{Z} \right)^{\top},$$

where W, X, Z are Gaussian with i.i.d. entries. (Gaussian Equivalence)

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- Extension to L layers: when $\theta_2(\sigma) = 0$, μ_L is Marchenko-Pastur.

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- Outliers depending on Hermite coefficients similar to [Fan-Montanari 19].
- Extension to *L* layers: when $\theta_2(\sigma) = 0$, μ_L is Marchenko-Pastur.
- Matched with [Fan-Wang 20] if XX^T has a Marchenko-Pastur distribution.

Question: a unified proof for two types of conditions on σ and W?

Spectrum of conjugate kernels, random data



Figure: [Benigni-Péché 21]

Neural tangent kernel

$$egin{aligned} &\mathcal{K}^{\mathsf{NTK}} := & (
abla_ heta f_ heta(X))^ op (
abla_ heta f_ heta(X)) \in \mathbb{R}^{n imes n} \ &= & X_L^ op X_L + \sum_{\ell=1}^L (S_\ell^ op S_\ell) \odot (X_{\ell-1}^ op X_{\ell-1}) \end{aligned}$$

When L = 1,

$$K^{\mathsf{NTK}} = X_1^\top X_1 + X^\top X \odot \left(\frac{1}{d_1} \sigma' (WX)^\top \operatorname{diag}(\mathbf{w})^2 \sigma' (WX)\right).$$

- Training errors evolved during gradient descent is governed by K^{NTK} . For $d_1 \rightarrow \infty$ and fixed *n*, K^{NTK} converges to its expectation and is fixed over training in the infinite width limit.
- The smallest singular value of K^{NTK} controls the global convergence of gradient descent.

[Jacot, Gabriel, Hongler 18], [Chizat et al 18], [Du et al 19], [Allen-Zhu et al 19], [Lee et al 19], [Arora et al 19], [Oymak-Soltanolkotabi 20], [Adlam et al 20], [Fan, Wang 20], [Montanari Zhong 22], [Bombari-Amani-Mondelli 22] ...

Random feature regression

A two-layer neural network $f : \mathbb{R}^d \to \mathbb{R}$ at random initialization

$$f(\mathbf{x}) = \frac{1}{\sqrt{n}} \boldsymbol{\theta}^{\top} \sigma(\mathbf{W} \mathbf{x}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{N} \boldsymbol{\theta}_{i} \sigma(\mathbf{w}_{i}^{\top} \mathbf{x}).$$

•
$$\boldsymbol{W} = \begin{bmatrix} \boldsymbol{w}_1^\top \\ \vdots \\ \boldsymbol{w}_N^\top \end{bmatrix} \in \mathbb{R}^{N \times d}$$
: weight matrix with i.i.d. $N(0, 1)$ entries.

• Training the output layer weight= linear regression with respect to random features $\phi(\mathbf{x}_i) = \sigma(\mathbf{W}\mathbf{x}_i) \in \mathbb{R}^N$.

[Ghorbani-Mei-Misiakiewicz-Montanari 21, Mei-Montanari 22, Misiakiewicz 22, Hu-Lu 22, Montanari-Zhong 22],...

Random feature ridge regression (RFRR) Training data $(\mathbf{x}_i, y_i), \dots, (\mathbf{x}_n, y_n), y_i = f_*(\mathbf{x}_i) + \varepsilon_i$.

• The loss function is defined by

$$L(\boldsymbol{\theta}) = \frac{1}{n} \|f(\boldsymbol{X}) - \boldsymbol{y}\|^2 + \frac{\lambda}{n} \|\boldsymbol{\theta}\|^2.$$

• Then the optimal predictor for RFRR is given by

$$\widehat{f}^{(\mathsf{RF})}_\lambda({m{x}}) = {m{\kappa}}_{\!N}({m{x}},{m{X}})({m{\kappa}}_{\!N}+\lambda \mathsf{Id})^{-1}{m{y}},$$

where K_N is the empirical *conjugate kernel matrix*:

$$\boldsymbol{K}_{N} = \frac{1}{N} \sigma \left(\boldsymbol{W} \boldsymbol{X} \right)^{\top} \sigma \left(\boldsymbol{W} \boldsymbol{X} \right) \in \mathbb{R}^{n \times n}.$$

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Training error:

$$E_{\mathsf{train}}^{(RF,\lambda)} := \frac{1}{n} \|\hat{f}_{\lambda}^{(RF)}(\boldsymbol{X}) - \mathbf{y}\|_2^2 = \frac{\lambda^2}{n} \|(\boldsymbol{K}_N + \lambda \mathsf{Id})^{-1} \mathbf{y}\|^2.$$

• *Test/ generalization error*: **x** sampled from the same distribution as training data,

$$\mathcal{R}(\hat{f}) := \mathbb{E}_{\mathbf{x}}[|\hat{f}(\mathbf{x}) - f^*(\mathbf{x})|^2].$$

Double descent for generalization error

[Mei-Montanari 22] (informal):

- Assume w_i, x_i are i.i.d. uniformly distributed on \mathbb{S}^{d-1} , $y_i = \langle \beta, x_i \rangle + \varepsilon_i$.
- $N/d \rightarrow \psi_1, n/d \rightarrow \psi_2$, $\lim_n \mathcal{R}(\hat{f})$ is a function of λ, ψ_1, ψ_2 and other model parameters.



Question: Universality for general weights/data distributions?

Kernel ridge regression

• Consider the empirical Risk Minimization (ERM)

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(\mathbf{x}_i))^2 + \lambda \|f\|_{\mathcal{H}},$$

where $\lambda \geq 0$ and \mathcal{H} is the Reproducing Kernel Hilbert Space for $k(\cdot, \cdot)$.

• Kernel ridge regression's predictor:

$$\widehat{f}_{\lambda}^{(\mathsf{K})}(oldsymbol{x}) = oldsymbol{\mathcal{K}}(oldsymbol{x},oldsymbol{\mathcal{X}})(oldsymbol{\mathcal{K}}(oldsymbol{X},oldsymbol{X}) + \lambda \mathsf{Id})^{-1}oldsymbol{y},$$

where $\boldsymbol{K}(\boldsymbol{x}, \boldsymbol{X}) = [k(\boldsymbol{x}, \boldsymbol{x}_1), \dots, k(\boldsymbol{x}, \boldsymbol{x}_1)]$ and $(\boldsymbol{K}(\boldsymbol{X}, \boldsymbol{X}))_{i,j} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ for $1 \leq i, j \leq n$ and $\boldsymbol{x}, \boldsymbol{x}_i \in \mathbb{R}^d$.

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• When $N \gg n$, random feature regression can be approximated by KRR.

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• When $N \gg n$, random feature regression can be approximated by KRR.

[Bartlett-Montanari-Rakhlin 21]: For $K_{ij} = f(\langle \mathbf{x}_i, \mathbf{x}_j \rangle / d)$, $n \simeq d$, KRR is asymptotically equivalent to linear ridge regression with a different ridge parameter.

proved for subgaussian data x_i with general covariance Σ .

Beyond $n \asymp d$, polynomial regime $n \asymp d^k$

- A simple example: when $f(x) = x^k$, $\mathcal{K}(x_i, x_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle^k = \langle \mathbf{x}_i^{\otimes k}, \mathbf{x}_j^{\otimes k} \rangle$.
- Let Y = [x₁^{⊗k}, · · · , x_n^{⊗k}] ∈ ℝ^{d^k×n}. Then K = Y[⊤]Y has a Marchenko-Pastur law when n ≍ d^k [Yaskov 23]. Connection to random tensor models [Bryson-Vershynin-Zhao 21].

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Universality [Lu-Yau 22, Dubova-Lu-McKenna-Yau 23]

 $f(x) = \sum_{k=0}^{L} c_k h_k(x)$. $\mathbf{K}_{ij} = \frac{1}{\sqrt{n}} f(\frac{1}{\sqrt{d}} \langle \mathbf{x}_i, \mathbf{x}_j \rangle) \mathbf{1}\{i \neq j\}$. $\frac{n}{d^{\ell}} \to \kappa > 0$. \mathbf{x}_i has i.i.d. entries with all finite moments.

- When ℓ is an integer, the limiting law is the free convolution of the semicirle law and Marchenko-Pastur law.
- \bullet When ℓ is not an integer, the limiting law is semicircle.

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 $f(x) = \sum_{k=0}^{L} c_k h_k(x)$. $\mathbf{K}_{ij} = \frac{1}{\sqrt{n}} f(\frac{1}{\sqrt{d}} \langle \mathbf{x}_i, \mathbf{x}_j \rangle) \mathbf{1}\{i \neq j\}$. $\frac{n}{d^{\ell}} \to \kappa > 0$. \mathbf{x}_i has i.i.d. entries with all finite moments.

- When ℓ is an integer, the limiting law is the free convolution of the semicirle law and Marchenko-Pastur law.
- \bullet When ℓ is not an integer, the limiting law is semicircle.

- A simple example: when $f(x) = x^k$, $K(x_i, x_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle^k = \langle \mathbf{x}_i^{\otimes k}, \mathbf{x}_j^{\otimes k} \rangle$.
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heuristics: When $\ell \in \mathbb{Z}$, $\mathbf{K} = \sum_{i=1}^{L} a_i \mathbf{K}_i$, each \mathbf{K}_i approximately independent. $\sum_{i=1}^{\ell-1} \mathbf{K}_i$ is low-rank, \mathbf{K}_{ℓ} has a Marchenko-Pastur law, $\sum_{i=\ell+1}^{L} a_i \mathbf{K}_i$ has a semicircle law.

Kernel regression in the polynomial regime [Xiao-Hu-Misiakiewicz-Lu-Pennington 22]

- When $n \simeq d^{\ell}, \ell \in \mathbb{Z}$, $\mathbf{x}_1, \ldots, \mathbf{x}_n$ i.i.d. uniformly on \mathbb{S}^{d-1} .
- *K_{ij}* = f((*x_i*, *x_j*)). Different scaling compared to [LY22, DLMY23]. *K* has a Marchenko-Pastur law. Generalization of [El Karoui 10].

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• Random feature regression $N \simeq d^{\kappa_1}$, $n \simeq d^{\kappa_2}$ [Hu-Lu-Misiakiewicz 24].

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 Nonlinear spiked covariance model and connection to neural networks [Ba-Erdogdu-Suzuki-Wang-Wu 23, Wang-Wu-Fan 24].

Other topics

- Feature learning with gradient descent [Ba-Murat-Erdogdu-Suzuki-Wang-Wu-Yang 22]
- Spectrum of empirical Hessian after SGD [Ben Arous-Gheissari-Huang-Jagannath 23]
- Generalization error of SGD in high dimensions [Paquette-Paquette-Adlam-Pennington 22]
- Gaussian equivalence [Hu-Lu 22], [Goldt-Loureiro-Reeves-Krzakala-Mzard-Zdeborová 21], [Montanari-Ruan-Saeed-Sohn 23],...
- Benign overfitting [Bartlett-Long-Lugosi-Tsigler 20], [Tsigler-Bartlett 23], [Koehler-Zhou-Sutherland-Srebro 21],...

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Let $p \in (0, 1)$ be fixed.

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Connected to TV distance between GOE(n) and Wishart(n, d) [Jiang-Li 15]. Detect local dependence by counting signed triangles.

- Question: Sparse regime $p = \frac{c}{n}$. $d \approx \log^3(n)$ is the conjectured threshold in [BDER16].
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- Spectral gap of **A** in certain regimes [Liu-Mohanty-Schramm-Yang 22, Bagachev-Bresler 24].
- Geometric block model: x_i, \ldots, x_n are drawn from a Gaussian mixture [Li-Schramm 24]. Testing geometry, community recovery/clustering.

Conclusions

- In the proportional regime $n \asymp d$, a nonlinear random matrix model behaves like another linear random matrix model.
- A polynomial regime n ≍ d^ℓ appears for nonlinear models, new phenomena in the spectrum and regression performance.
- Question: Universality and structured data for generalization error.
- Question: spectrum of geometric random graphs.