Inference from heterogeneous pairwise data

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August 2023

Pairwise inference model

- Latent variables $(x_1, \ldots, x_N) \in \mathcal{X}^N$.
- lacktriangleright Observations through memoryless channel P with input alphabet $\mathcal{X} \times \mathcal{X}$

$$Y_{ij} \stackrel{\mathsf{ind}}{\sim} P(\cdot \mid x_i, x_j), \quad i, j = 1, \dots N$$

Spin glasses



Sherrington-Kirkpatrick model (with planted signal)

$$Y_{ij} \sim \mathsf{N}\Big(\sqrt{\frac{\lambda}{N}}x_ix_j, 1\Big), \quad \lambda \ge 0, \quad x_i \in \{\pm 1\}$$

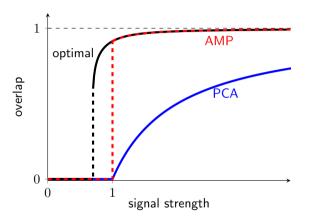
Stochastic block model

$$Y_{ij} \sim \mathsf{Bern}(Q_{x_i,x_j}), \quad Q \in [0,1]^{K \times K}, \quad x_i \in \{1,\dots,K\}$$

Spiked covariance model

$$Y_{ij} \sim \mathsf{N}\Big(\sqrt{\frac{\lambda}{N}}\langle u_i, v_j \rangle, 1\Big), \quad \lambda \ge 0, \qquad u_i, v_j \in \mathbb{R}^r$$

Statistical & computational limits



Why mutual information?

$$I(\mathbf{X}; \mathbf{Y}) = D(P_{XY} \parallel P_X \otimes P_Y) = \int dP_{XY} \log \frac{dP_{XY}}{d(P_X \otimes P_Y)}$$

I-MMSE relationship: If $X \in \mathbb{R}^{N \times d}$ then

$$\frac{d}{dt}I\big(\boldsymbol{X};\boldsymbol{Y},\sqrt{t}\boldsymbol{X}+\boldsymbol{Z}\big)\Big|_{t=0} = \mathbb{E}\big[\|\boldsymbol{X}-\mathbb{E}[\boldsymbol{X}\mid\boldsymbol{Y}]\|_F^2\big]$$
 where $\boldsymbol{Z}\in\mathbb{R}^{N\times d}\perp\!\!\!\perp(\boldsymbol{X},\boldsymbol{Y})$ has IID standard Gaussian entries.

Hence, formula for asymptotic mutual information (with side information) gives formula for asymptotic minimum mean square error almost everywhere*.

* Limit is not differentiable at phase transitions

Channel universality

Classical scaling (fixed p large n) Local asymptotic normality & Fisher information

$$\log \frac{dP_{n,\theta+\epsilon_n u}}{dP_{n,\theta}} \quad \xrightarrow[n\to\infty]{} \quad \log \frac{dQ_u}{dQ_0}, \qquad \underbrace{Q_u = \mathsf{N}(I_\theta u, I_\theta)}_{\text{Gaussian model}}$$

High-dimensional scaling Korada-Montanari 2011, Deshpande-Abbe-Montanari 2015 Krzakala-Xu-Zdeborová 2016, Lesieur-Krzakala-Zdeborová 2017, R.-Mayya-Volfovsky 2019 Guionnet-Ko-Krzakala-Zdeborová 2023

Compare free energy / mutual information for prior distribution π on θ

$$\left| \mathbb{E}_{P_{\theta}} \log \int \frac{dP_{n,\theta+r_n u}}{dP_{n,\theta}} \pi(du) - \mathbb{E}_{Q_0} \log \int \frac{dQ_u}{dQ_0} \pi(du) \right| = o(n)$$

Gaussian comparison holds for dense SBM but not for sparse SBM

Model for Today's talk

- Assume \mathcal{X} is (or can be embedded into) a subset of \mathbb{R}^d . (d is fixed)
- $X = (x_1, \dots, x_N)^{\top}$ is $N \times d$ matrix with IID rows & finite fourth moments.

Family of channels
$$(P_N)_{N\in\mathbb{N}}$$
. Approximate by linear Gaussian model
$$P_N(\cdot\mid x_i,x_j) \quad \approx \quad \mathsf{N}\Big(\sqrt{\frac{1}{N}}\,B^\top(x_i\otimes x_j),\mathrm{I}_L\Big), \quad B\in\mathbb{R}^{d^2\times L}$$

Includes bounded degree polynomials in Gaussian noise via lifting

$$f(\theta_i, \theta_j) = b^{\top}(x_i \otimes x_j), \qquad x_i = (1, \theta_i, \theta_i^2, \dots \theta_i^{d-1})^{\top}$$

Includes groupwise heteroskedasticity via augmentation

$$x_i = \underbrace{(0, \dots, \theta_i, \dots, 0)^{\top}}_{\text{position indexed by group}}$$

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Entropy / free energy with IID prior

ightharpoonup Rows of $X \in \mathbb{R}^{n \times d}$ are IID copies of $X_0 \in \mathbb{R}^d$ with finite fourth moments.

$$D(\boldsymbol{Y} \parallel \boldsymbol{Z}) = \underbrace{\mathbb{E}\bigg[\log \int e^{\langle \boldsymbol{x}^{\otimes 2}B, \boldsymbol{Y} \rangle - \frac{1}{2} \|\boldsymbol{x}^{\otimes 2}B\|_F^2} P_0^{\otimes N}(d\boldsymbol{x})\bigg]}_{\text{original problem is } N \times d}, \quad \boldsymbol{Y} = \boldsymbol{X}^{\otimes 2}B + \boldsymbol{Z}$$

 $lackbox{Entropy function } \mathcal{D} \colon \mathbb{S}^d_+ o [0,\infty) \text{ defined by }$

$$\begin{split} \mathcal{D}(R) &\coloneqq D\big(R^{1/2}X_0 + Z_0 \parallel Z_0\big), \\ &= \underbrace{\mathbb{E}\bigg[\log \int e^{\langle x, RX_0 + Z_0 \rangle - \frac{1}{2}x^\top Rx} P_0(dx)\bigg]}_{\text{easy problem is } d \times 1}, \quad X_0 \; \perp \!\!\! \perp \; Z_0 \sim \mathsf{N}(0, I_d) \end{split}$$

Symmetric spiked matrix model

$$\frac{1}{N}D(\boldsymbol{Y} \parallel \boldsymbol{G}) \xrightarrow{N \to \infty} \max_{Q \in \mathbb{S}_+^d} \left\{ \mathcal{D}(Q) - \frac{1}{4\lambda} \operatorname{tr}(Q^2) \right\}$$

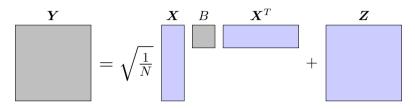
- Rank-one: Deshpande et al. 2015, Krzakala-Xu 2016, Barbier et al. 2016
- ▶ finite rank: Lelarge, Miolane 2017

Asymmetric spiked matrix model

$$\frac{1}{N}D(\boldsymbol{Y}\parallel\boldsymbol{Z})\xrightarrow{N\to\infty}\max_{Q_1\in\mathbb{S}_+^d}\min_{Q_2\in\mathbb{S}_+^d}\left\{\mathcal{D}_1(Q_2)+\mathcal{D}_2(Q_1)-\frac{1}{2\lambda}\operatorname{tr}(Q_1Q_2)\right\}$$

- ► Rank-one: Barbier et al. 2017
- ▶ finite rank: Miolane 2017

Spiked matrix model with coupling matrix



- ▶ Deterministic coupling matrix $B \in \mathbb{R}^{d \times d}$
- ► Stochastic block model with general interactions R.-Mayya-Volvosky 2019

Includes previous models as special cases:

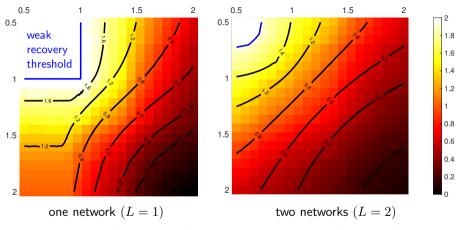
- lacktriangle Symmetric spiked model \iff B is positive (or negative) semidefinite
- lacktriangle Asymmetric spiked model \iff augmentation + asymmetric B

Multiview spiked matrix model

- Applied to community detection with correlated networks by Mayya-R. 2019 who proved lower bound on the asymptotic free energy.
- ▶ Matching upper bound by Barbier-R. 2020 under structural assumption

$$\sum_{\ell=1}^{L} \{ (B_{\ell} \otimes B_{\ell}) + (B_{\ell} \otimes B_{\ell})^{\top} \} \succeq 0.$$

Community detection with correlated networks [Mayya-R. 2019]



Asymptotic MMSE (contour lines) vs. empirical MSE of BP (heat map). Networks have $N=10^5$ nodes, 3 communities, and average degree 30. Axes are eigenvalues of first coupling matrix.

Assumption on the coupling matrices in [Barbier-R. 2020] is restrictive

$$\sum_{\ell=1}^{L} \{ (B_{\ell} \otimes B_{\ell}) + (B_{\ell} \otimes B_{\ell})^{\top} \} \succeq 0.$$

- Cannot apply to asymmetric model or directed networks
- Formula for asymptotic MMSE is incorrect if assumption is violated.

Is there a universal formula that holds for arbitrary coupling matrices?

Matrix tensor product model

$$Y = \frac{1}{\sqrt{N}}(X \otimes X)B + Z$$

- $ightharpoonup X \otimes X$ is $N^2 \times d^2$ Kronecker product
- ightharpoonup B is $d^2 \times L$ coupling matrix
- **Equivalent** to multiview model with matrices B_1, \ldots, B_L via

$$B = \begin{bmatrix} \mathsf{vec}(B_1) & \dots & \mathsf{vec}(B_L) \end{bmatrix}$$

Theorem [R. 2020] For any coupling matrix
$$B$$
,
$$\frac{1}{N}D(\boldsymbol{Y}\parallel\boldsymbol{Z})\xrightarrow{N\to\infty}\max_{Q\in\mathbb{S}^d_+}\inf_{R\in\mathbb{S}^d_+}\left\{\mathcal{D}(R)+\frac{1}{2}\operatorname{tr}(BB^\top(Q\otimes Q))-\frac{1}{2}\operatorname{tr}(RQ)\right\}$$
 Bound on convergence rate is $O(d^4N^{-1/5})$.

Relation with previous work

▶ Structural assumption in [Barbier, R. 2020] is equivalent to convexity of

$$Q \mapsto \operatorname{tr}(BB^{\top}(Q \otimes Q))$$

▶ If convexity holds, then max-min formula reduces to simplified max formula

$$\max_{Q \in \mathbb{S}_+^d} \inf_{R \in \mathbb{S}_+^d} \left\{ \mathcal{D}(R) + \frac{1}{2} \operatorname{tr}(BB^\top (Q \otimes Q)) - \frac{1}{2} \operatorname{tr}(RQ) \right\}$$
$$= \max_{Q \in \mathbb{S}_+^d} \left\{ \mathcal{D}(T(Q)) - \frac{1}{2} \operatorname{tr}(BB^\top (Q \otimes Q)) \right\}$$

where $T \colon \mathbb{S}^d \to \mathbb{S}^d$ is self-adjoint linear operator defined by B.

Why this formula?

Augmented model: Given $(R,S) \in \mathbb{S}^d \times \mathbb{S}^{d^2}$ define

$$m{Y} = egin{cases} rac{1}{\sqrt{N}} m{X}^{\otimes 2} S^{1/2} + m{Z}, & ext{MTP model} \ m{X} m{R}^{1/2} + m{Z}' & ext{linear Gaussian model} \end{cases}$$

$$\mathcal{D}_N(R,S) \coloneqq rac{1}{N} D(oldsymbol{Y} \, \| \, \mathsf{IID} \, \, \mathsf{Gaussian})$$

Overlap concentration implies matching of derivatives

$$2
abla_S \mathcal{D}_N = \mathbb{E}ig[(rac{1}{N}oldsymbol{X}^ op ilde{oldsymbol{X}})^{\otimes 2}ig] pprox ig(\mathbb{E}ig[rac{1}{N}oldsymbol{X}^ op ilde{oldsymbol{X}}ig]ig)^{\otimes 2} = ig(2
abla_R \mathcal{D}_Nig)^{\otimes 2}$$

Heuristic derivation (assuming overlap concentration)

$$\mathcal{D}_N^*(Q,S) \coloneqq \sup_R \underbrace{\left\{\frac{1}{2}\langle R,Q\rangle - \mathcal{D}_N(R,S)\right\}}_{\text{convex conjugate in 1st arg.}}$$

$$\nabla_S \mathcal{D}_N^*(Q,S) = -\nabla_S \mathcal{D}(R^*(Q),S) \overset{\text{overlap conc.}}{\approx} -2 \big(\nabla_R \mathcal{D}(R^*(Q),S)\big)^{\otimes 2} = -\frac{1}{2} Q^{\otimes 2}$$

$$\mathcal{D}_N^*(Q, S) \approx \mathcal{D}_N^*(Q, 0) - \frac{1}{2} \langle S, Q^{\otimes 2} \rangle$$
 (*)

$$\underbrace{ \mathcal{D}_N(0,S)}_{\text{original problem}} = \underbrace{\sup_{Q} \{ \langle 0,Q \rangle - \mathcal{D}^*(Q,S) \}}_{\text{biconjugate in 1st arg.}} \overset{(\star)}{\approx} \sup_{Q} \left\{ \langle 0,Q \rangle - \mathcal{D}^*(Q,0) + \frac{1}{2} \langle S,Q^{\otimes 2} \rangle \right\}$$

$$= \sup_{Q} \inf_{R} \left\{ \mathcal{D}(R) + \frac{1}{2} \langle S,Q^{\otimes 2} \rangle - \langle R,Q \rangle \right\}$$

Main ideas in proof

- ► Start with adaptive interpolation method [Barbier-Macris 2018]
- Lack of convexity complicates specification of adaptive path
- ▶ Rely heavily on order-preserving properties of overlap in Gaussian noise.
- ▶ Introduce continuous time variance inequality linking free energy and overlap.

Higher order tensor products?

$$oldsymbol{Y} = rac{1}{\sqrt{N^{p-1}}} oldsymbol{X}^{\otimes p} B + oldsymbol{Z}$$

Applying result for p=2 recursively suggests following formula

$$\frac{1}{N}D(\boldsymbol{Y} \parallel \boldsymbol{Z}) \xrightarrow{N \to \infty} \max_{Q \in \mathbb{S}_+^d} \min_{R \in \mathbb{S}_+^d} \left\{ \mathcal{D}_0(R) + \frac{1}{2} \langle BB^\top, Q^{\otimes p} \rangle - \frac{1}{2} \langle R, Q \rangle \right\}$$

This formula proved via Hamilton-Jacobi equations by Chen-Mourrat-Xia 2021

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Pairwise observations through channel P with input alphabet $\mathcal{X} \times \mathcal{X}$

$$Y_{ij} \stackrel{\mathsf{ind}}{\sim} P(\cdot \mid x_i, x_j), \quad i, j = 1, \dots N$$

- What if there are different types of variables?
- ▶ What if the observations depend on the variable type?

Groupwise spiked matrix model

- Latent variables partitioned in K groups.
- Obtain pairwise observations for each group

$$oldsymbol{Y}_{k\ell} = \sqrt{rac{\lambda_{k\ell}}{N}} oldsymbol{X}_k oldsymbol{X}_\ell^ op + oldsymbol{Z}_{k\ell}, \qquad k,\ell = 1,\ldots,K$$

where X_k is $n_k \times 1$ vector of variables in k-th group.

Theorem [Behne-R. 2022] If
$$n_k/N \to \beta_k > 0$$
 and k -th group IID P_k ,
$$\frac{1}{N}D(\boldsymbol{Y} \parallel \boldsymbol{Z}) \xrightarrow{N \to \infty} \max_{q \succeq 0} \inf_{r \succeq 0} \left\{ \sum_{k=1}^K \mathcal{D}_k(r_k) + \frac{1}{2} \sum_{k,\ell=1}^K \lambda_{k\ell} \, q_k q_\ell - \frac{1}{2} r^\top q \right\}$$

Related recent work by Guionnet-Ko-Krzakala-Zdeborová

Special cases depend on which interactions are observed

$$\Lambda = \begin{pmatrix} \lambda_{11} & \dots & \lambda_{1K} \\ \vdots & & \vdots \\ \lambda_{K1} & \dots & \lambda_{KK} \end{pmatrix}$$

- ► One nonzero (diagonal) ⇒ symmetric spiked matrix model
- ▶ One nonzero (off-diagonal) ⇒ asymmetric spiked matrix model
- ► Off-diagonal row ⇒ generalized spiked covariance model [Bai-Yao 2012]
- ► Two nonzeros (one diagonal, one off-diagonal) ⇒ Gaussian version of the contextual stochastic block model (SBM) [Deshpande-Montanari-Mossel-Sen 2018]
- ► Family of doubly stochastic Toeplitz matrices ⇒ Proof technique called spatial coupling. Used to study spiked Wigner model [Barbier et al. 2018]
- ▶ Tri-diagonal matrix \implies Used to analyze free energy in deep Boltzmann machine with K layers [Albericiet al. 2021]

Implications for weighted PCA

 Heteroskedastic spiked covariance model: Samples from p-variate Gaussian with covariance

$$\Sigma = \sqrt{rac{\lambda}{N}} oldsymbol{x} oldsymbol{x}^ op + \underbrace{\Sigma_0}_{\mathsf{diagona}}$$

• Overlap of optimally weighted PCA when diagonal entries of Σ_0 are supported on a finite set $\{\sigma_1^2, \ldots, \sigma_L^2\}$, Hong et al. 2018

$$\frac{\langle \boldsymbol{x}, \hat{\boldsymbol{x}} \rangle^2}{\|\boldsymbol{x}\|^2 \|\hat{\boldsymbol{x}}\|^2} \xrightarrow[n \to \infty]{\text{a.s.}} \quad \text{largest real root of } R(z) \coloneqq 1 - \sum_{\ell=1}^L \frac{\beta_\ell}{\sigma_\ell^2} \frac{1-z}{\sigma_\ell^2 + z}$$

Theorem [Behne-R. 2022]

The weighted PCA method of Hong et al. 2018 is information-theoretically optimal for a spherical spike.

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Joint with with Riccardo Rossetti



AMP for low-rank + IID Gaussian noise

$$oldsymbol{Y} = rac{1}{n} oldsymbol{X} oldsymbol{X}^{ op} + rac{1}{\sqrt{n}} \mathsf{GOE}$$

- ► Low-rank Lesieur-Krzakala-Zdeborová 2017, Montanari-Venkataramanan 2021
- Non-separable denoisers Berthier-Montanari-Nguyen 2020

Matrix-valued AMP with non-separable denoisers: Gerbelot-Berthier 2021

- ▶ Sequence of Lipschitz denoisers: f_t : $\mathbb{R}^{N \times d} \to \mathbb{R}^{N \times d}$
- lacktriangle Initialize $oldsymbol{X}_0 \in \mathbb{R}^{N imes d}$ and iterate

$$m{M}_t = f_t(m{X}_t), \qquad m{D}_t = rac{1}{N} \sum_{i=1}^N rac{\partial f_{ti}}{\partial m{x}_{ti}}(m{X}_t)$$

$$\boldsymbol{X}_{t+1} = \boldsymbol{Y}\boldsymbol{M}_t - \boldsymbol{M}_{t-1}\boldsymbol{D}_t$$

State evolution with non-separable denoisers

State Evolution: Define $m{X}_t^* \sim \mathsf{N}(m{X}K_t, \Sigma_t \otimes \mathrm{I}_N)$ recursively via

$$K_0 = \frac{1}{n} \mathbb{E} \big[\boldsymbol{X}^{\top} f_0(\boldsymbol{X}_0) \big], \qquad \Sigma_0 = \frac{1}{n} \mathbb{E} \big[f_0(\boldsymbol{X}_0)^{\top} f_0(\boldsymbol{X}_0) \big]$$

$$K_{t+1} = \frac{1}{n} \mathbb{E} \big[\boldsymbol{X}^{\top} f_t(\boldsymbol{X}_t^*) \big], \qquad \Sigma_{t+1} = \frac{1}{n} \mathbb{E} \big[f_t(\boldsymbol{X}_t^*)^{\top} f_t(\boldsymbol{X}_t^*) \big]$$

Theorem: Gerbelot-Berthier 2021 Under regularity conditions, for all uniformly pseudo-Lipschitz $\phi_N \colon \mathbb{R}^{N \times d} \to \mathbb{R}$

$$\left|\phi_N(\underbrace{X,X_0,\dots,X_t}_{\text{amp iterations}}) - \mathbb{E}\,\phi_N\underbrace{(X,X_0^*,\dots,X_t^*)}_{\text{state evolution}}\right| \xrightarrow[N \to \infty]{\text{pr}} 0$$

AMP for MTP model

$$Y_{\ell} = \frac{1}{n} X B_{\ell} X^{\top} + \frac{1}{\sqrt{n}} Z_{\ell}, \quad \ell = 1, \dots, L$$

AMP for MTP: Rossetti-R.

- ▶ Sequence of Lipschitz denoisers: f_t : $\mathbb{R}^{n \times d} \to \mathbb{R}^{n \times d}$,
- lacktriangle Initialize $oldsymbol{X}_0 \in \mathbb{R}^{n imes d}$ and iterate

$$oldsymbol{M}_t = f_t(oldsymbol{X}_t) \qquad oldsymbol{D}_t = rac{1}{n} \sum_{i=1}^n rac{\partial f_{ti}}{\partial oldsymbol{x}_{ti}}(oldsymbol{X}_t)$$

$$oldsymbol{X}_{t+1} = \sum_{\ell=1}^L oldsymbol{Y}_\ell oldsymbol{M}_t A_{t\ell}^ op + oldsymbol{Y}_\ell^ op oldsymbol{M}_t A_{t\ell} - oldsymbol{M}_{t-1} (oldsymbol{A}_{t\ell} oldsymbol{D}_t A_{t\ell}^ op + oldsymbol{A}_{t\ell}^ op oldsymbol{D}_t A_{t\ell})$$

Theorem: Optimal reweighting $\iff A_{t\ell} = B_{\ell}$ for all ℓ, t .

State evolution under optimal reweighting

State Evolution: Define $m{X}_t^* \sim \mathsf{N}(m{X}K_t, \Sigma_t \otimes \mathrm{I}_n)$ recursively via

$$K_0 = \frac{1}{n} \boldsymbol{X}^{\top} f_0(\boldsymbol{X}_0), \qquad \Sigma_0 = \frac{1}{n} f_0(\boldsymbol{X}_0^{\top}) f_0(\boldsymbol{X}_0)$$

$$K_{t+1} = T \left(\frac{1}{n} \mathbb{E} \left[\boldsymbol{X}^{\top} f_t(\boldsymbol{X}_t^*) \right] \right), \qquad \Sigma_{t+1} = T \left(\frac{1}{n} \mathbb{E} \left[f_t(\boldsymbol{X}_t^*)^{\top} f_t(\boldsymbol{X}_t^*) \right] \right)$$

$$T(S) = \sum_{\ell} B_{\ell} S B_{\ell}^{\top} + B_{\ell}^{\top} S B_{\ell}$$

Linear operator $T \colon \mathbb{R}^{d \times d} \to \mathbb{R}^{d \times d}$ is self-adjoint and completely positive

Theorem: SE for Bayes-optimal AMP defined by \mathbb{S}^d_+ -valued recursion

$$S_{t+1} = T(2\nabla \mathcal{D}(S))$$

Fixed-points \iff Stationary point of IT potential

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- ► G, Reeves, Information-theoretic limits for the matrix tensor product, *IEEE Journal on Selected Areas in Information Theory*, 2020
- ▶ J. K. Behne and G. Reeves, Fundamental limits for rank-one matrix estimation with groupwise heteroskedasticity, *AISTATS*, 2023
- ▶ R. Rossetti and G. Reeves, Heteroskedastic Low-rank Matrix Factorization [Arxiv, 2023] See poster this evening

Summary and future directions

Pairwise inference model

$$Y_{ij} \stackrel{\mathsf{ind}}{\sim} P_N(\cdot \mid x_i, x_j), \quad i, j = 1, \dots N$$

MTP model

$$P_N(\cdot \mid x_i, x_j) \quad \approx \quad \mathsf{N}\Big(\sqrt{\frac{1}{N}} \, B^\top(x_i \otimes x_j), \mathsf{I}_L\Big), \quad B \in \mathbb{R}^{d^2 \times L}$$

Further directions

- ► Weak recovery / BBP phase transitions
- ► Non-Gaussian observations + channel universality
- Spectral methods
- Coupling matrices are unknown, mismatched estimation
- Extrinsic rank, higher-order interactions