A few challenges in large-rank matrix denoising and factorization

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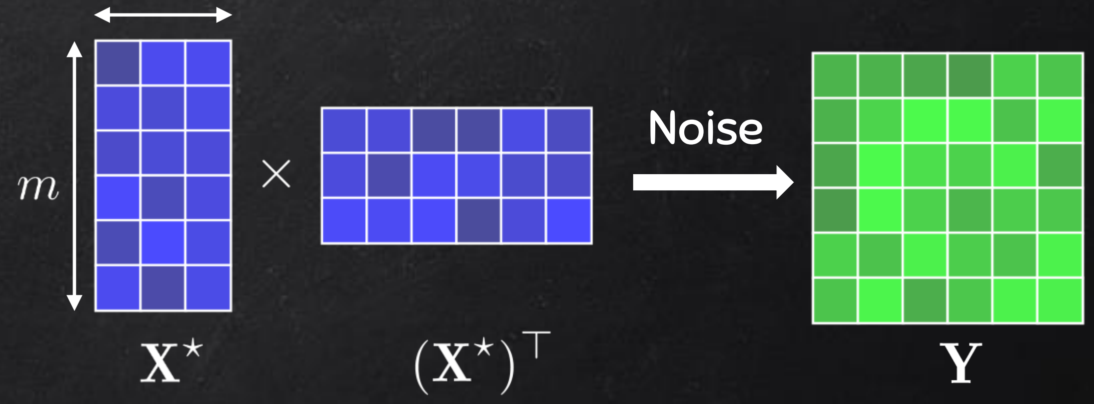
Setting

[M., Krzakala, Mézard & Zdeborová '22]

$$Y_{\mu\nu} \sim P_{\text{out}}\Big(\cdot \,\Big|\, \frac{1}{\sqrt{n}} \sum_{i=1}^{n} X^\star_{\mu i} X^\star_{\nu i}\Big)$$

$\mathbf{X}^\star \sim P_X$



Task

Recover $\mathbf{X}^\star$ — Factorization

Recover $\mathbf{S}^\star = \mathbf{X}^\star(\mathbf{X}^\star)^\top$ — Denoising

Dictionary learning, sparse coding, sparse PCA, matrix completion...

Setting:

- High-dimensional: $m \to \infty$
- P_X, P_{out} are known ➡ $\hat{\mathbf{S}}(\mathbf{Y}) = \mathbb{E}[\mathbf{S}|\mathbf{Y}]$

Minimal Mean Squared Error estimator

$\mathrm{MMSE} = \mathbb{E}\|\mathbb{E}[\mathbf{S}|\mathbf{Y}] - \mathbf{S}^\star\|_F^2$

- Large m limit ?
- Reachable by efficient algorithms ?

✓ $n = \mathcal{O}(1)$ (low-rank).

[Rangan&al'12], [Deshpande&al'14], [Lesieur&al '15], [Perry&al'16], [Lelarge&al'19], [Aubin, M.,&al '20] ....

Here $m/n = \alpha \in (0, \infty)$

This talk

Denoising ➕ $X_{\mu i} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0,1)$

Generalizations

Other models for $\mathbf{S}$, non-symmetric factorization $\mathbf{Y} \sim P_{\text{out}}(\mathbf{UV})$, ...

Rotationally-invariant denoising (1)

[Ledoit & Péché '11]
[Bun, Allez, Bouchaud & Potters '16]

Assume noise is additive and rotationally-invariant

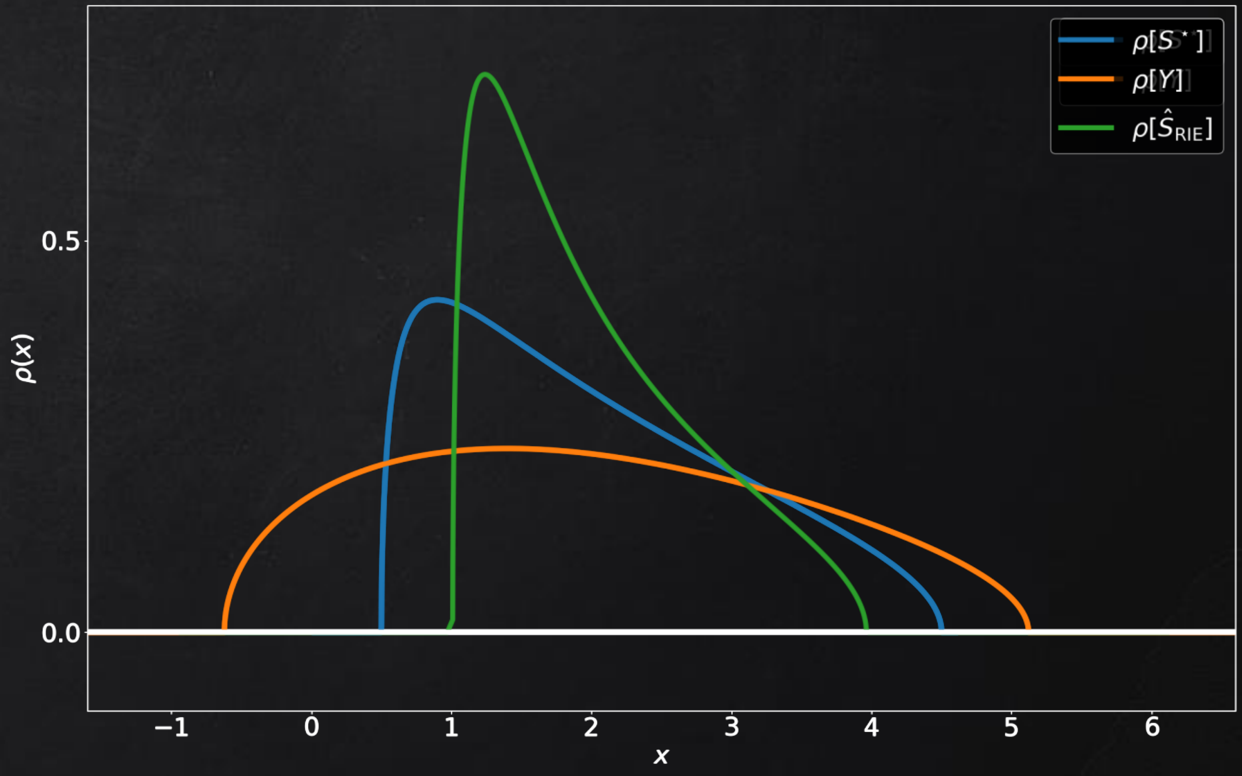
$$\boxed{\mathbf{Y} = \mathbf{S}^\star + \sqrt{\Delta}\mathbf{Z}}$$ → Gaussian (GOE) noise

Rotationally-invariant estimator (RIE) $\hat{\mathbf{S}}_{\rm RIE} = \sum_{\mu=1}^{m} \hat{\xi}_\mu \mathbf{u}_\mu \mathbf{u}_\mu^\top$ → Eigenvectors of $\mathbf{Y}$

$$\hat{\xi}_\mu = \arg\min_{\boldsymbol{\xi}\in\mathbb{R}^m} \|\mathbf{S}^\star - \hat{\mathbf{S}}(\boldsymbol{\xi})\|_F^2$$

Eigenvalues of $\mathbf{Y}$

$$\boxed{\hat{\xi}_\mu = y_\mu - 2\Delta \times \mathrm{P.P.}\int \rho_{\mathbf{Y}}(\mathrm{d}t)\frac{1}{t - y_\mu}}$$



"Miraculous solution": only depends on the spectral properties of $\mathbf{Y}$

Easily computed with tools of free probability [Voiculescu, ...]

Rotationally-invariant denoising (2)

$$\mathbf{Y} = \mathbf{S}^\star + \sqrt{\Delta}\mathbf{Z}$$

$$\mathbb{P}(\mathbf{S}|\mathbf{Y}) = \frac{1}{\mathcal{Z}(\mathbf{Y})} P^{(\alpha)}_{\mathrm{Wish.}}(\mathbf{S}) \exp\left\{-\frac{1}{4\Delta}\|\mathbf{Y}-\mathbf{S}\|_F^2\right\} \propto P^{(\alpha)}_{\mathrm{Wish.}}(\mathbf{S}) \exp\left\{-\frac{\|\mathbf{S}\|_F^2}{4\Delta} + \frac{1}{2\Delta}\mathrm{Tr}[\mathbf{YS}]\right\}$$

$$f(\mathbf{ODO}^\top) = f(\mathbf{D}) \Rightarrow \mathbb{E}[f(\mathbf{S})|\mathbf{Y}] = \int_{\mathbb{R}^m} \mathrm{d}\mathbf{D}\, q(\mathbf{D})\, f(\mathbf{D}) \int_{\mathcal{O}(m)} \mathcal{D}\mathbf{O} \exp\left\{\frac{1}{2\Delta}\mathrm{Tr}\left[\mathbf{YODO}^\top\right]\right\}$$

"HCIZ" integral [Harish-Chandra-Itzykson-Zuber]

$$\boxed{\int_{\mathcal{O}(m)} \mathcal{D}\mathbf{O} \exp\left\{m\mathrm{Tr}\left[\mathbf{AO}\mathbf{B}\mathbf{O}^\top\right]\right\}}$$

Full-rank

known for $m \to \infty$

- When $\mathrm{rank}(\mathbf{A}) = o(m)$ [Guionnet '05]
- When $\mathrm{rank}(\mathbf{A}) = \Theta(m)$ [Matytsin '94, Guionnet&al '02]

[M., Krzakala, Mézard & Zdeborová '22]

- Analytical formula $\mathrm{MMSE} = \int \rho_{\mathbf{Y}}(\mathrm{d}t)\,(\cdots)$ cf also [Pourkamali, Barbier & Macris '23]
- Re-derivation of the optimal RIE estimator as $\hat{\mathbf{S}}_{\mathrm{opt.}} = \mathbb{E}[\mathbf{S}|\mathbf{Y}] \simeq \hat{\mathbf{S}}_{\mathrm{RIE}}$

Estimator and asymptotic characterization extend to the non-symmetric setting [Erba, Troiani, Krzakala, M. & Zdeborová '22]

Beyond rotation invariant denoising

[M., Krzakala, Mézard & Zdeborova '22]

$$Y_{\mu\nu} \sim P_{\rm out}(\cdot|S^\star_{\mu\nu})$$

$$\mathbf{S}^\star = \frac{1}{\sqrt{n}}\mathbf{X}^\star(\mathbf{X}^\star)^\top$$

- Exact characterization of the MMSE ✗
- Efficient optimal estimator ✗

Unknown

Proposed Approximate Message Passing (AMP) algorithms

→ Convergence problems + hard-to-control assumptions

[Kabashima & al '16, Parker &al '14, Zou & al '21, Lucibello & al '21]

This talk: sketch a perturbative approach to clarify these difficulties, and lay a path for improvement.

$$S_{\mu\nu} = \frac{1}{\sqrt{n}}\sum_{i=1}^n x_{\mu i}x_{\nu i}$$

$H_{\mu\nu}$: conjugate field

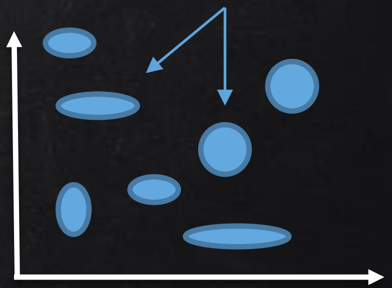
$$\mathbb{P}(\mathbf{X}|\mathbf{Y}) = \frac{1}{\mathcal{Z}(\mathbf{Y})}\prod_{\mu,i} p_X(x_{\mu i})\prod_{\mu,\nu} P_{\rm out}\left(Y_{\mu\nu}\middle|\frac{1}{\sqrt{n}}\sum_{i=1}^n x_{\mu i}x_{\nu i}\right)$$

$$P(\mathbf{X},\mathbf{H}) \propto \left[\prod_{\mu,i} p_X(x_{\mu i})\right]\left[\prod_{\mu,\nu} Q(Y_{\mu\nu},H_{\mu\nu})\right]\exp\left\{\frac{1}{\sqrt{n}}\sum_{i,\mu,\nu} H_{\mu\nu}x_{\mu i}x_{\nu i}\right\}$$

"Effective" distribution

Plefka–Georges–Yedidia expansion

"Pure states"

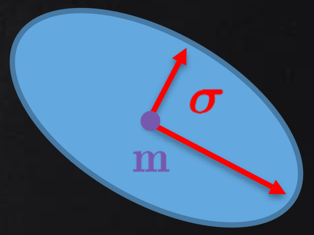


Idea: $P(\mathbf{X},\mathbf{H}) \propto \left[\prod_{\mu,i} p_X(x_{\mu i})\right]\left[\prod_{\mu,\nu} Q(Y_{\mu\nu},H_{\mu\nu})\right] \exp\left\{\frac{\eta}{\sqrt{n}}\sum_{i,\mu,\nu} H_{\mu\nu}x_{\mu i}x_{\nu i}\right\}$

Thouless-Anderson-Palmer approximation [TAP77]

There is a function $\Phi_{\mathrm{TAP}}(\mathbf{m},\boldsymbol{\sigma})$ whose maxima give the "pure states" in which $P(\mathbf{X},\mathbf{H})$ concentrates its mass.

TAP free energy

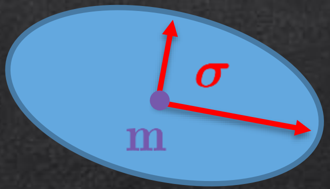


Worked out in spin glass models and simpler statistical inference models [Parisi&Potters '95], [M.&al '19]

$$\Phi_{\mathrm{TAP}}(\mathbf{m},\boldsymbol{\sigma}) = \sum_{k=0}^{\infty} \frac{\partial_\eta^k \Phi_{\mathrm{TAP}}(\mathbf{m},\boldsymbol{\sigma})[\eta=0]}{k!}$$

- $\partial_k^\eta \Phi_{\mathrm{TAP}}(\mathbf{m},\boldsymbol{\sigma})[\eta=0]$ can be recursively computed by the "PGY" method [Plefka '82, Georges&Yedidia '91]
- It turns out that (at least for the first orders) "$\eta \Leftrightarrow \sqrt{m/n} = \sqrt{\alpha}$": "overcomplete" limit $\mathbf{S}^\star \simeq \mathrm{I}_m + \varepsilon(\alpha)$.

The PGY expansion



$$\mathbf{m} = (m_{\mu\nu})$$

$$\boldsymbol{\sigma} = \mathrm{Diag}(\{\sigma_{\mu\nu}\})$$

PGY

$$\Phi_{\mathrm{TAP}}(\mathbf{m},\boldsymbol{\sigma}) = \sum_{\mu,\nu} \Big[\operatorname*{extr}_{\boldsymbol{\omega},\mathbf{b}} \Big\{ -\omega_{\mu\nu} m_{\mu\nu} - \frac{b_{\mu\nu}}{2}\big(-\sigma_{\mu\nu}^2 + m_{\mu\nu}^2\big) + \ln \int \mathrm{d}z \, \frac{e^{-\frac{1}{2b_{\mu\nu}}(z-\omega_{\mu\nu})^2}}{\sqrt{2\pi b_{\mu\nu}}} P_{\mathrm{out}}(Y_{\mu\nu}|z) \Big\} \Big]$$

$$+\frac{\eta^2}{2}\sum_{\mu,\nu}[m_{\mu\nu}^2 - \sigma_{\mu\nu}^2] + \frac{\eta^3}{6n^{1/2}} \sum_{\substack{\mu_1,\mu_2,\mu_3 \\ \text{pairwise distinct}}} m_{\mu_1\mu_2} m_{\mu_2\mu_3} m_{\mu_3\mu_1} + \mathcal{O}(\eta^4)$$

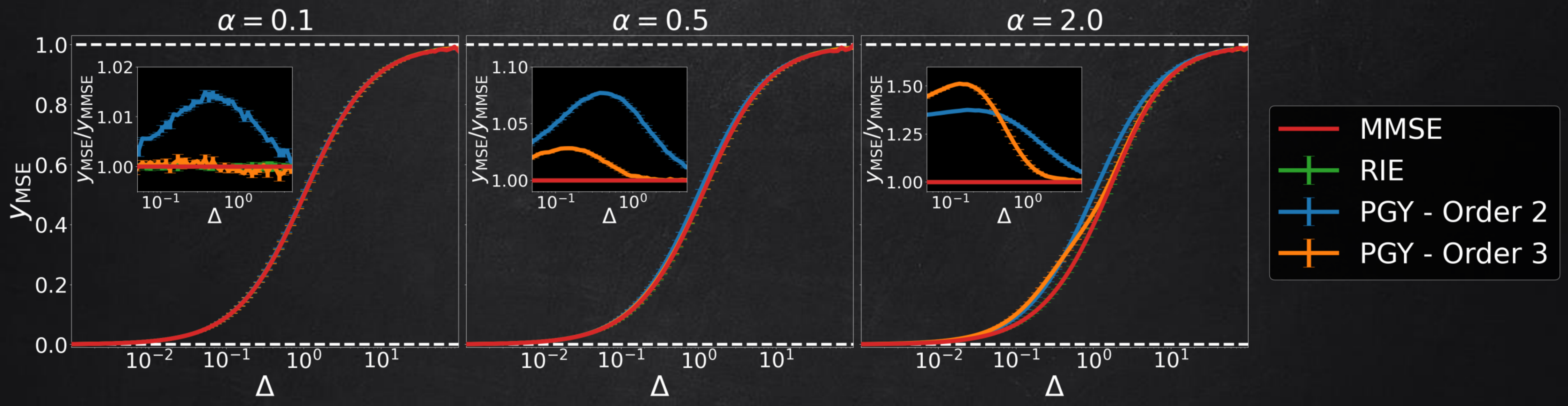
- Iterative equations to find the maxima of Φ_{TAP} can be turned into an algorithm [M., Foini, &al '19]
- Truncating at order η^2 $\Longleftrightarrow$ "AMP" algorithms of [Kabashima & al'16, …]

  → We explicit their approximation
- However, order η^3 and above are <u>not negligible</u>

  → [Kabashima & al'16, …] effectively neglect some 3rd order correlations

Numerics for Gaussian denoising

$$\mathbf{Y} = \frac{\mathbf{X}^\star (\mathbf{X}^\star)^\intercal}{\sqrt{n}} + \sqrt{\Delta}\mathbf{Z} \quad ; \quad m = \alpha n$$



- "PGY order 3" significantly improves over order 2, in the overcomplete regime $\alpha \ll 1$.
- Analytical check that $\hat{\mathbf{S}}_{\mathrm{PGY}} \simeq \mathbb{E}[\mathbf{S}|\mathbf{Y}]$ up to order $(\sqrt{\alpha})^3$ ✓

Limitation of the PGY method

Orders 1, 2, 3, … of the expansion ⇒ Educated conjecture about arbitrary orders

For orders ≥ 4, PGY expansion becomes very tedious, need more investigation !

Conclusion

Some (of the many) open directions

- PGY expansion at orders ≥ 4 ? Arbitrary orders ? Possible resummation of the series ?
- Efficient denoising/factorization algorithms when $n = \Theta(m)$ and for non-RI noise ? $Y_{\mu\nu} \sim P_{\rm out}(\cdot|\sqrt{m}S^{\star}_{\mu\nu})$
- Transition between low-rank and extensive-rank regimes when rotationally-invariant :

$$I(\mathbf{A}) = \frac{1}{m^2} \log \int_{\mathcal{O}(m)} \mathcal{D}\mathbf{O} \exp\left\{m \mathrm{Tr}\left[\mathbf{AOBO}^\top\right]\right\} \qquad \mathrm{rank}(A) = o(m) \longleftrightarrow \mathrm{rank}(A) = \Theta(m)$$

?

[Alice Guionnet, "Rare events in Random Matrix theory", ICM 2022]

Other recent works: [Camilli & Mézard '23, Barbier & Macris '23, Pourkamali & Macris '23, Landau, Mel & Ganguli '23]

THANK YOU !