# From Spectral Estimators to Approximate Message Passing... And Back

Marco Mondelli

Institute of Science and Technology Austria (ISTA)

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Institute of Science and Technology Austria


SOMETIMES
THEY COME
BACK

# Credits

Andrea Montanari (Stanford)

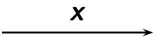
Ramji Venkataramanan (Cambridge)

Yihan Zhang (ISTA)

Hong Chang Ji (ISTA)

# From **Spectral Estimators** to Approximate Message Passing. . . And Back

# Generalized linear models

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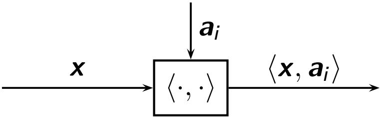


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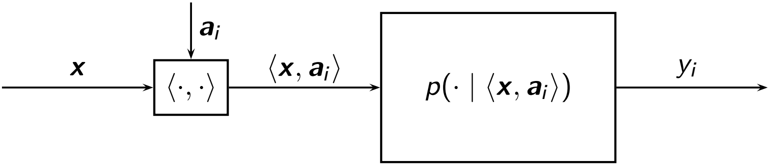


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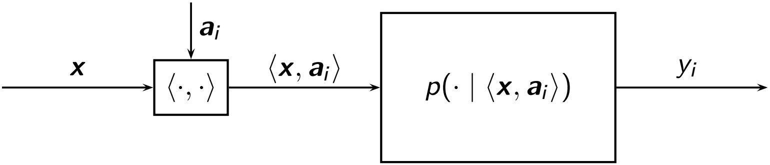


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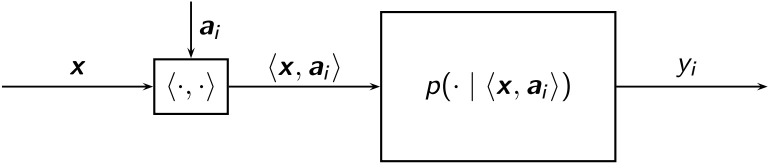
- **High-dimensional** regime: $n, d \to \infty$ and $n/d \to \delta \in (0, \infty)$.

# Spectral initialization




Most algorithms are iterative and require an **initialization**, often given by a spectral estimator:

$$\boldsymbol{D}_n = \frac{1}{n}\sum_{i=1}^{n} \mathcal{T}(y_i)\boldsymbol{a}_i\boldsymbol{a}_i^{\mathsf{T}}, \quad \hat{\boldsymbol{x}}^{\mathrm{s}} = \text{ principal eigenvector of } \boldsymbol{D}_n.$$

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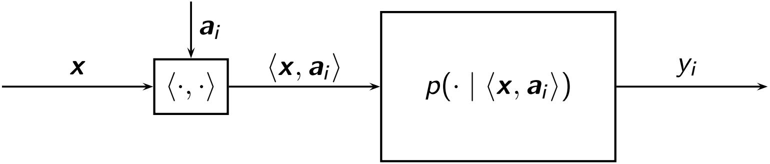


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- $\mathcal{T} : \mathbb{R} \to \mathbb{R}$ pre-processing function.

**Key questions**

- What's the performance of $\hat{\boldsymbol{x}}^{\mathrm{s}}$ (e.g., in terms of $\frac{|\langle \hat{\boldsymbol{x}}^{\mathrm{s}}, \boldsymbol{x} \rangle|}{\|\hat{\boldsymbol{x}}^{\mathrm{s}}\| \cdot \|\boldsymbol{x}\|}$)?
- What's the optimal $\mathcal{T}$?

# Phase transition for random matrices

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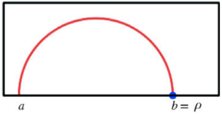


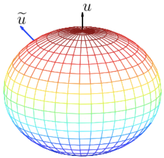

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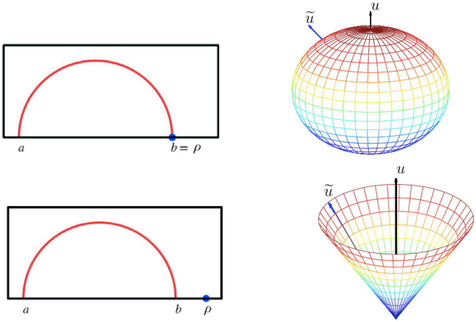


[BGN11]

**Eigenvalue gap $\Rightarrow$ eigenvector correlation**

# Phase transition for spectral algorithm

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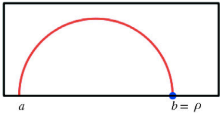


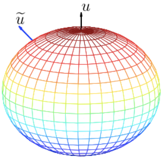


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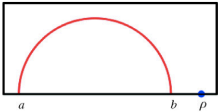


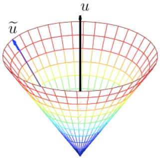


**Reduction to a rank-1 perturbation**

# Precise asymptotics for spectral estimators

**Theorem**

Let $\{\boldsymbol{a}_i\}_{1\le i\le n} \sim_{\text{i.i.d.}} \mathsf{N}(\boldsymbol{0}_d, \boldsymbol{I}_d/d)$. If $F(\delta,\mathcal{T}) > 0$, then:

1. **Spectral gap:** the limits of the top two eigenvalues of $\boldsymbol{D}_n$ are $\lambda_1(\delta,\mathcal{T}) > \lambda_2(\delta,\mathcal{T})$.
2. **Spectral estimator works:** $\lim_{n\to\infty} \frac{|\langle \hat{\boldsymbol{x}}^{\text{s}}, \boldsymbol{x}\rangle|}{\|\hat{\boldsymbol{x}}^{\text{s}}\| \cdot \|\boldsymbol{x}\|} = \rho(\delta,\mathcal{T}) > 0.$

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Explicit expressions for $\rho(\delta,\mathcal{T}), F(\delta,\mathcal{T}), \lambda_1(\delta,\mathcal{T}), \lambda_2(\delta,\mathcal{T})$

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- Precise asymptotics allow to optimize $\mathcal{T}$ [LL17, MM18, LAL19]

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- [DMM20, DBMM20, MDX+21] consider a Haar matrix $\boldsymbol{A}$.

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# How to solve phase retrieval?

Most algorithms are iterative and require an **initialization**:

- Approximate message passing [Ran11, SR15]
- Alternating minimization [NJS13]
- Wirtinger flow [CLS15]
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- Many many more. . . [FS20]

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# Generalized Approximate Message Passing (GAMP)

$$\boldsymbol{u}^t = \frac{1}{\sqrt{\delta}}\boldsymbol{A} f_t(\boldsymbol{v}^t) - \mathsf{b}_t g_{t-1}(\boldsymbol{u}^{t-1}; \boldsymbol{y})$$
$$\boldsymbol{v}^{t+1} = \frac{1}{\sqrt{\delta}}\boldsymbol{A}^\mathsf{T} g_t(\boldsymbol{u}^t; \boldsymbol{y}) - \mathsf{c}_t f_t(\boldsymbol{v}^t)$$

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- $f_t$ and $g_t$ Lipschitz and acting component-wise
- $\mathsf{b}_t = \frac{1}{n} \sum_{i=1}^d f_t'(v_i^t)$, $\mathsf{c}_t = \frac{1}{n} \sum_{i=1}^n g_t'(u_i^t; y_i)$

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## Theorem [Ran11, JM13]

The empirical joint distribution of $(\boldsymbol{u}^t, \boldsymbol{v}^t)$ converges to the law of

$$(U_t, V_t) \triangleq (\mu_{U,t} G + \sigma_{U,t} W_{U,t}, \mu_{V,t} X + \sigma_{V,t} W_{V,t}),$$

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- **Deterministic scalar** recursion for $\{\mu_{U,t}, \mu_{V,t}, \sigma_{U,t}, \sigma_{V,t}\}_{t\geq 1}$.
- **Bayes-optimal** (unless statistical-to-computational barrier) [BKM$^+$19].

# Spectral initialization of AMP

**Key difficulty**

Spectral initialization depends on the design matrix $\boldsymbol{A}$: AMP and SE need to be changed accordingly.

- Low-rank matrix estimation in [MV21a] (different approach)
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Design and analyze an **artificial AMP**

[MV21b] M. Mondelli and R. Venkataramanan, "Approximate Message Passing with Spectral Initialization for Generalized Linear Models", *AISTATS 2021 & JSTAT 2022*.

# Artificial AMP

**[Phase #1]** Iterates of artificial AMP approach $\hat{\boldsymbol{x}}^{\rm s}$ via **power method**.

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**[Phase #2]** Iterates of artificial AMP **mimic** iterates of true AMP.

# Artificial AMP as a power method

**[Phase #1]** Iterates of artificial AMP approach $\hat{\boldsymbol{x}}^{\mathrm{s}}$ via **power method**.

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Choose $f_t, g_t$ so that

$$\boldsymbol{v}^{t+1} \propto \boldsymbol{D}_n \boldsymbol{v}^t, \qquad \text{with } \boldsymbol{D}_n = \frac{1}{n}\sum_{i=1}^{n} \mathcal{T}(y_i)\boldsymbol{a}_i\boldsymbol{a}_i^{\mathsf{T}}$$

- As $t \to \infty$, $\boldsymbol{v}^t$ aligned with $\mathrm{eig}(\boldsymbol{D}_n)$

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Spectral gap proved in [MM18]!


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# Towards heterogeneous and correlated data

So far, estimation of single signal $\boldsymbol{x}$ via design matrix $\boldsymbol{A}$ i.i.d. Gaussian

- In practice, data are heterogeneous $\Longrightarrow$ **mixed GLMs**
- In practice, data have correlations $\Longrightarrow$ **structured GLMs**

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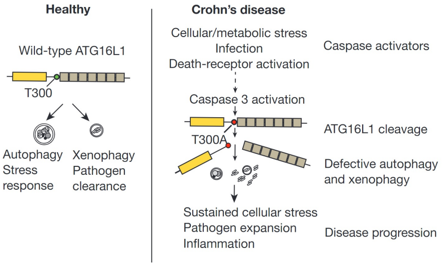
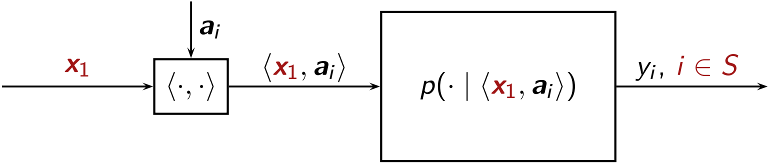
Example: Genome-Wide Association Studies (GWAS)

- Discovering novel biological mechanisms [MLP+14]
- Advancement in clinical care (validating new disease biomarkers, personalized medicine)



# Mixed generalized linear models



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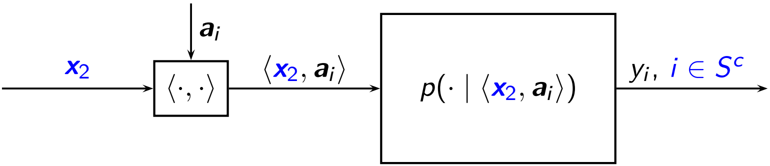

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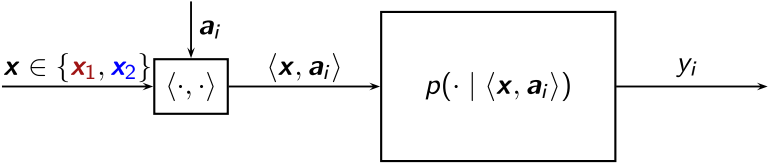


- Signals to **recover** $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^d$.
- **Known** sensing vector $\boldsymbol{a}_i$, $i \in [n]$.
- **Unknown** (latent) variables $\eta_i$, $i \in [n]$.
- Measurement $y_i \sim p(\cdot \mid \eta_i \langle \boldsymbol{x}_1, \boldsymbol{a}_i \rangle + (1 - \eta_i) \langle \boldsymbol{x}_2, \boldsymbol{a}_i \rangle)$, $i \in [n]$.
- **High dimensional** regime: $n, d \to \infty$ and $n/d \to \delta \in (0, \infty)$.

Model data **heterogeneity**, with applications in biology, physics, and economics [MP04, GL07, LSL19, DGP20].

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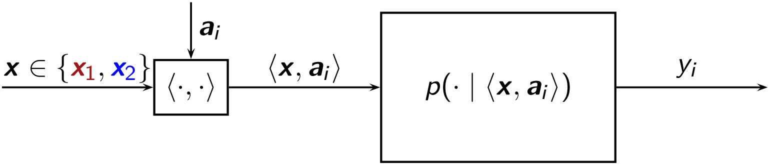


- $\boldsymbol{x}_1, \boldsymbol{x}_2$ i.i.d. and uniform on the sphere with radius $\sqrt{d}$.
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**Spectral estimator:**

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- $\mathcal{T} : \mathbb{R} \to \mathbb{R}$ pre-processing function.

# Precise asymptotics for spectral estimators

**Theorem [ZMV22]**

Let $\boldsymbol{x}_1, \boldsymbol{x}_2$ be i.i.d. and uniform on the sphere, and $\{\boldsymbol{a}_i\}_{1\le i\le n} \sim_{\text{i.i.d.}} \mathsf{N}(\boldsymbol{0}_d, \boldsymbol{I}_d/d)$. If $F_1(\delta, \mathcal{T}) > 0$, then

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If $F_2(\delta, \mathcal{T}) > 0$, then

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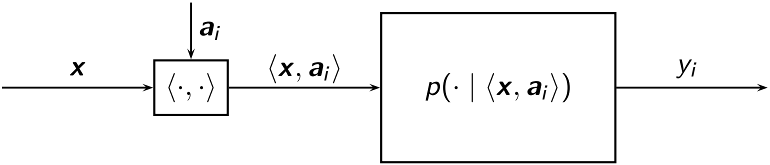
Explicit expressions for $\rho_1(\delta, \mathcal{T}), F_1(\delta, \mathcal{T})$, $\rho_2(\delta, \mathcal{T}), F_2(\delta, \mathcal{T})$.

- **Optimize** $\mathcal{T}$ both in terms of spectral threshold and overlap.

[ZMV22] Y. Zhang, M. Mondelli, and R. Venkataramanan, "Precise Asymptotics for Spectral Methods in Mixed Generalized Linear Models", *arXiv:2211.11368*, 2022.

# Generalized linear models with general Gaussian design




- $\boldsymbol{x}$ with i.i.d. zero-mean unit-variance components.
- $\{\boldsymbol{a}_i\}_{1 \le i \le n} \sim_{\text{i.i.d.}} \mathsf{N}(\mathbf{0}_d, \boldsymbol{\Sigma}/n)$.
- High dimensional regime: $n, d \to \infty$ and $n/d \to \delta \in (0, \infty)$.

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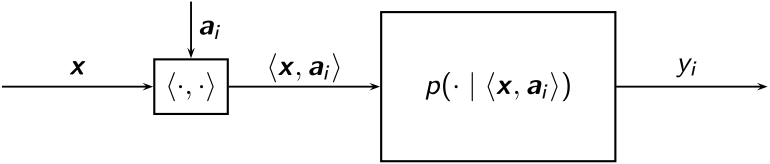


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Anisotropic covariates commonly seen in practice, but existing work mostly focuses on penalized regression [W09, GBRD14, JM14, ZZ14, JM18, ZSC22].

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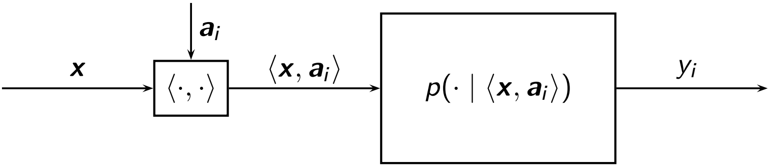


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**Spectral estimator:**

$$\boldsymbol{D}_n = \frac{1}{n} \sum_{i=1}^{n} \mathcal{T}(y_i) \boldsymbol{a}_i \boldsymbol{a}_i^{\mathsf{T}}, \quad \hat{\boldsymbol{x}}^{\mathrm{s}} = \text{ top eigenvector of } \boldsymbol{D}_n$$

- $\mathcal{T} : \mathbb{R} \to \mathbb{R}$ pre-processing function.

# Precise asymptotics for spectral estimators

**Theorem [ZJVM23]**

Let $\boldsymbol{x}$ have i.i.d. zero-mean unit-variance components, and $\{\boldsymbol{a}_i\}_{1\leq i\leq n} \sim_{\text{i.i.d.}} \mathrm{N}(\mathbf{0}_d, \boldsymbol{\Sigma}/n)$. Assume $\mathcal{T}$ is Lipschitz and satisfies some mild regularity conditions. If $F(\delta, \Sigma, \mathcal{T}) > 0$, then:

1. **Spectral gap:** the limits of the top two eigenvalues of $\boldsymbol{D}_n$ are $\lambda_1(\delta, \Sigma, \mathcal{T}) > \lambda_2(\delta, \Sigma, \mathcal{T})$.
2. **Spectral estimator works:** $\lim_{n\to\infty} \frac{|\langle \hat{\boldsymbol{x}}^{\mathrm{s}}, \boldsymbol{x}\rangle|}{\|\hat{\boldsymbol{x}}^{\mathrm{s}}\| \cdot \|\boldsymbol{x}\|} = \rho(\delta, \Sigma, \mathcal{T}) > 0.$

Explicit expressions for $\rho(\delta, \Sigma, \mathcal{T}), F(\delta, \Sigma, \mathcal{T}), \lambda_1(\delta, \Sigma, \mathcal{T}), \lambda_2(\delta, \Sigma, \mathcal{T})$.

[ZJVM23] Y. Zhang, H. C. Ji, R. Venkataramanan, and M. Mondelli, "Spectral Estimators for Structured Generalized Linear Models via Approximate Message Passing", *arXiv:2308.14507*, 2023.

# Optimal spectral methods for general Gaussian designs

**Theorem [ZJVM23]**

If $\delta > \delta^*(\Sigma)$, then there is $\mathcal{T}^*(\Sigma)$ s.t. spectral estimator works. Otherwise, under an additional technical assumption, there is no $\mathcal{T}$ s.t. $F(\delta, \Sigma, \mathcal{T}) > 0$.

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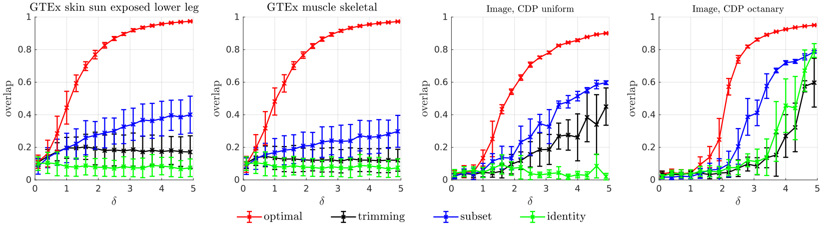
- $\mathcal{T}^*(\Sigma)$ depends on $\Sigma$ only via its **trace** (which can be estimated consistently).
- This **proves conjecture** of [MKLZ22] for class of spectral distributions of $\boldsymbol{A}$.
- $\delta^*(\Sigma)$ **meets information-theoretic** weak recovery **limit** conjectured in [MLKZ20].

# Universality of the optimal $\mathcal{T}^*(\Sigma)$

- $\boldsymbol{x}$ uniform on the sphere.
- $\boldsymbol{A}$ taken from datasets popular in quantative genetics (GTEx) and computational imaging (CDP).
- $y_i = |\langle \boldsymbol{x}, \boldsymbol{a}_i \rangle|$.




**Significant improvement** over heuristic choices of $\mathcal{T}$

# Challenges

Mixed GLMs: we characterize eigenvalues with free probability tools, but unclear how to study eigenvectors...

Structured GLMs: unclear even how to characterize eigenvalues...

# Challenges and ideas

Mixed GLMs: we characterize eigenvalues with free probability tools, but unclear how to study eigenvectors...

Structured GLMs: unclear even how to characterize eigenvalues...

**New strategy** to analyze spectral methods based on **Approximate Message Passing (AMP)**

# AMP as a power method

Choose $f_t, g_t$ so that

$$\boldsymbol{v}^{t+1} \propto \boldsymbol{D}_n \boldsymbol{v}^t, \qquad \text{with } \boldsymbol{D}_n = \frac{1}{n}\sum_{i=1}^{n} \mathcal{T}(y_i)\boldsymbol{a}_i\boldsymbol{a}_i^{\mathsf{T}}$$

- As $t \to \infty$, $\boldsymbol{v}^t$ aligned with $\mathrm{eig}(\boldsymbol{D}_n)$ if $\boldsymbol{D}_n$ has a **spectral gap**

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Mixed GLMs: we characterize eigenvalues ($\Rightarrow$ spectral gap) with free probability tools and **eigenvectors via AMP**

Structured GLMs: we characterize $\ell_2$-**norm of AMP iterates** to unveil spectral gap

# AMP iterates

$$\boldsymbol{v}^{t+1} = \frac{\boldsymbol{D}_n}{\gamma}\boldsymbol{v}^t + \boldsymbol{e}^t$$

- $\lim_{t\to\infty}\lim_{d\to\infty}\|\boldsymbol{e}^t\|^2/d = 0$

# AMP iterates

$$\boldsymbol{v}^{t+1} = \frac{\boldsymbol{D}_n}{\gamma}\boldsymbol{v}^t$$

# AMP iterates

$$\boldsymbol{v}^{t+t'} = \left( \frac{\boldsymbol{D}_n}{\gamma} \right)^{t'} \boldsymbol{v}^t$$

# $\ell_2$-norm of AMP iterates

$$\frac{1}{d}\|\boldsymbol{v}^{t+t'}\|^2 = \frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{v}^t\right\|^2$$

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$$= \left(\lambda_1\left(\frac{\boldsymbol{D}_n}{\gamma}\right)\right)^{2t'}\frac{\langle \boldsymbol{v}_1(\boldsymbol{D}_n), \boldsymbol{v}^t\rangle^2}{d}$$

$$+ \frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{\Pi}\boldsymbol{v}^t\right\|^2$$

- $\boldsymbol{\Pi}$ projector orthogonal to top eigenvector

# $\ell_2$-norm of AMP iterates

$$\begin{aligned}\frac{1}{d}\|\boldsymbol{v}^{t+t'}\|^2 &= \frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{v}^t\right\|^2\\ &= \left(\lambda_1\left(\frac{\boldsymbol{D}_n}{\gamma}\right)\right)^{2t'}\frac{\langle \boldsymbol{v}_1(\boldsymbol{D}_n), \boldsymbol{v}^t\rangle^2}{d}\\ &\quad + \frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{\Pi}\boldsymbol{v}^t\right\|^2\end{aligned}$$

$$\frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{\Pi}\boldsymbol{v}^t\right\|^2 \le \left(\lambda_2\left(\frac{\boldsymbol{D}_n}{\gamma}\right)\right)^{2t'}\frac{1}{d}\|\boldsymbol{v}^t\|^2$$

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# $\ell_2$-norm of AMP iterates

$$\lim_{t'\to\infty}\lim_{t\to\infty}\lim_{d\to\infty}\frac{1}{d}\|\boldsymbol{v}^{t+t'}\|^2 = \frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{v}^t\right\|^2$$

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- $\lim_{d\to\infty}$ allows to apply **state evolution**
- $\lim_{t\to\infty}$ gives the **fixed point**
- $\lim_{t'\to\infty}$ boosts the **spectral gap**

# $\ell_2$-norm of AMP iterates

$$\lim_{t'\to\infty}\lim_{t\to\infty}\lim_{d\to\infty}\frac{1}{d}\|\boldsymbol{v}^{t+t'}\|^2 = \frac{1}{d}\left\|\left(\frac{\boldsymbol{D}_n}{\gamma}\right)^{t'}\boldsymbol{v}^t\right\|^2$$

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Provided that $\lim_{d\to\infty}\lambda_2(\boldsymbol{D}_n) < \gamma$

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1. Guess the correct value of $\gamma$
2. Compute edge of the bulk and verify that $\lim_{d\to\infty} \lambda_2(\boldsymbol{D}_n) < \gamma$
3. Deduce that

$$\lim_{t'\to\infty} \lim_{t\to\infty} \lim_{d\to\infty} \left(\lambda_1\left(\frac{\boldsymbol{D}_n}{\gamma}\right)\right)^{2t'} \frac{\langle \boldsymbol{v}_1(\boldsymbol{D}_n), \boldsymbol{v}^t\rangle^2}{d} = \lim_{t'\to\infty} \lim_{t\to\infty} \lim_{d\to\infty} \frac{1}{d}\|\boldsymbol{v}^{t+t'}\|^2 := \rho^2$$

4. Conclude that

$$\lim_{d\to\infty} \lambda_1(\boldsymbol{D}_n) = \gamma \text{ (outlier)}$$

$$\lim_{t\to\infty} \lim_{d\to\infty} \frac{\langle \boldsymbol{v}_1(\boldsymbol{D}_n), \boldsymbol{v}^t\rangle^2}{d} = \rho^2 \text{ (overlap)}$$

# Conclusions

Analysis based on AMP **broadly applicable**:

- Rotationally invariant designs
- Matrix estimation with heteroscedastic/correlated noise
- Universality of spectral estimators
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Thank you for your attention!