# Low-rank Matrix Estimation via Approximate Message Passing

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**WoLA 2018**

# The Spiked Model

$$A = \sum_{i=1}^{k} \lambda_i v_i v_i^{\mathsf{T}} + W \qquad \in \mathbb{R}^{n \times n}$$

- $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_k$ are deterministic scalars
- $v_1, \ldots, v_k \in \mathbb{R}^n$ are orthonormal vectors
- $W \sim \mathrm{GOE}(n) \quad \Rightarrow \quad W$ symmetric with $(W_{ii})_{i \leq n} \sim_{i.i.d.} \mathrm{N}(0, \frac{2}{n})$ and $(W_{ij})_{i<j \leq n} \sim_{i.i.d.} \mathrm{N}(0, \frac{1}{n})$

GOAL: To estimate the vectors $v_1, \ldots, v_k$ from $A$

# Spectrum of spiked matrix

$$\boldsymbol{A} = \sum_{i=1}^{k} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^{\mathsf{T}} + \boldsymbol{W}$$

Random matrix theory and the 'BBAP' phase transition :

- Bulk of eigenvalues of $\boldsymbol{A}$ in $[-2, 2]$ distributed according to Wigner's semicircle
- Outlier eigenvalues corresponding to $|\lambda_i|$'s greater than 1:

$$z_i \to \lambda_i + \frac{1}{\lambda_i} > 2$$

- Eigenvectors $\boldsymbol{\varphi}_i$ corresponding to outliers $z_i$ satisfy

$$|\langle \boldsymbol{\varphi}_i, \boldsymbol{v}_i \rangle| \to \sqrt{1 - \lambda_i^{-2}}$$

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[Baik, Ben Arous, Péché '05], [Baik, Silverstein '06], [Capitaine, Donati-Martin, Féral '09], [Benaych-Georges and Nadakuditi '11], ...

# Structural information

$$\boldsymbol{A} = \sum_{i=1}^{k} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^{\mathsf{T}} + \boldsymbol{W}$$

When $\boldsymbol{v}_i$'s are unstructured, e.g., drawn uniformly at random from the unit sphere,

- Best estimator of $\boldsymbol{v}_i$ is the $i$th eigenvector $\boldsymbol{\varphi}_i$
- If $|\lambda_i| \geq 1$, then $|\langle \boldsymbol{v}_i, \boldsymbol{\varphi}_i \rangle| \to \sqrt{1 - \frac{1}{\lambda_i^2}}$

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But we often have *structural* information about $\boldsymbol{v}_i$'s

- For example, $\boldsymbol{v}_i$'s may be sparse, bounded, non-negative etc.
- Relevant for many applications: sparse PCA, non-negative PCA, community detection under stochastic block model, ...
- Can improve on spectral methods

# Prior on eigenvectors

$$\boldsymbol{A} = \sum_{i=1}^{k} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^{\mathsf{T}} + \boldsymbol{W} \equiv \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{\mathsf{T}} + \boldsymbol{W}$$

$$\boldsymbol{V} = [\boldsymbol{v}_1 \ \boldsymbol{v}_2 \ldots \boldsymbol{v}_k] \quad \mathbb{R}^{n\times k}$$

If each row of $\boldsymbol{V}$ is $\sim_{i.i.d}$ $P_{\underline{V}}$, then Bayes-optimal estimator (for squared error) is

$$\widehat{\boldsymbol{V}}_{\text{Bayes}} = \mathbb{E}\left[\boldsymbol{V} \mid \boldsymbol{A}\right]$$

- Generally not computable
- Closed-form expressions for asymptotic Bayes error

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[Deshpande, Montanari '14], [Barbier *et al.* '16], [Lesieur *et al.* '17], [Miolane, Lelarge '16] ...

# Computable estimators

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- Convex relaxations generally do not achieve Bayes optimal error [Javanmard, Montanari, Ricci-Tersinghi '16]
- MCMC can approximate Bayes estimator, but can have very large mixing time and hard to analyze

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**In this talk**

Approximate Message Passing (AMP) algorithm to estimate $\boldsymbol{V}$

# Rank one spiked model

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}, \qquad \boldsymbol{v} \sim_{i.i.d.} P_V, \quad \mathbb{E}V^2 = 1$$

Power iteration for principal eigenvector:

$\boldsymbol{x}^{t+1} = \boldsymbol{A}\boldsymbol{x}^t$, with $\boldsymbol{x}^0$ chosen at random

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**AMP**:

$$\boldsymbol{x}^{t+1} = \boldsymbol{A}\, f_t(\boldsymbol{x}^t) - \mathrm{b}_t f_{t-1}(\boldsymbol{x}^{t-1}), \qquad \mathrm{b}_t = \frac{1}{n}\sum_{i=1}^{n} f_t'(x_i^t)$$

- Non-linear function $f_t$ chosen based on structural info on $\boldsymbol{v}$
- Memory term ensures a nice distributional property for the iterates in high dimensions
- Can be derived via approximation of belief propagation equations

# State evolution

$$\boldsymbol{x}^{t+1} = \boldsymbol{A}\, f_t(\boldsymbol{x}^t) - \mathrm{b}_t f_{t-1}(\boldsymbol{x}^{t-1}), \quad \text{with } \mathrm{b}_t = \frac{1}{n}\sum_{i=1}^{n} f_t'(x_i^t)$$

If we initialize with $\boldsymbol{x}^0$ *independent* of $\boldsymbol{A}$, then as $n \to \infty$:

$$\boldsymbol{x}^t \longrightarrow \mu_t \boldsymbol{v} + \sigma_t \mathbf{g}$$

- $\mathbf{g} \sim_{i.i.d.} \mathrm{N}(0,1)$, independent of $\boldsymbol{v} \sim_{i.i.d.} P_V$

[Bayati,Montanari '11], [Rangan, Fletcher '12], [Deshpande, Montanari '14]

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- $\mathbf{g} \sim_{i.i.d.} \mathrm{N}(0,1)$, independent of $\boldsymbol{v} \sim_{i.i.d.} P_V$
- Scalars $\mu_t, \sigma_t^2$ recursively determined as

$$\mu_{t+1} = \lambda\, \mathbb{E}[V\, f_t(\mu_t V + \sigma_t G)], \quad \sigma_{t+1}^2 = \mathbb{E}[f_t(\mu_t V + \sigma_t G)^2]$$

- Initialize with $\mu_0 = \frac{1}{n}|\mathbb{E}\langle \boldsymbol{x}^0, \boldsymbol{v}\rangle|$

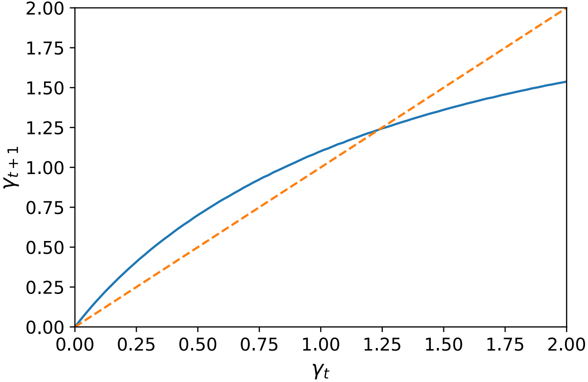
[Bayati,Montanari '11], [Rangan, Fletcher '12], [Deshpande, Montanari '14]

# Bayes-optimal AMP

Assuming $\boldsymbol{x}^t = \mu_t \boldsymbol{v} + \sigma_t \mathbf{g}$, choose $f_t(y) = \mathbb{E}[V \mid \mu_t V + \sigma_t G = y]$

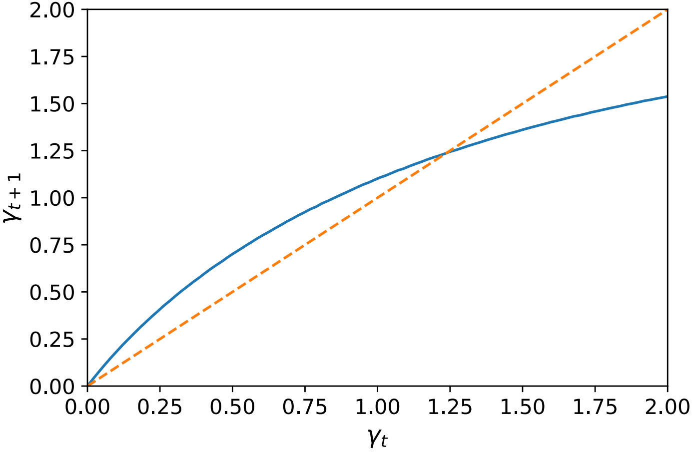
State evolution becomes $\gamma_{t+1} = \lambda^2\{1 - \mathrm{mmse}(\gamma_t)\}$ with $\mu_t = \sigma_t^2 = \gamma_t$

$P_V \sim \text{uniform}\{1, -1\}, \quad \lambda = \sqrt{2}$




Initial value $\gamma_0 \propto \frac{1}{n}|\mathbb{E}\langle \boldsymbol{x}^0, \boldsymbol{v}\rangle|$, what is $\lim_{t\to\infty} \gamma_t$?

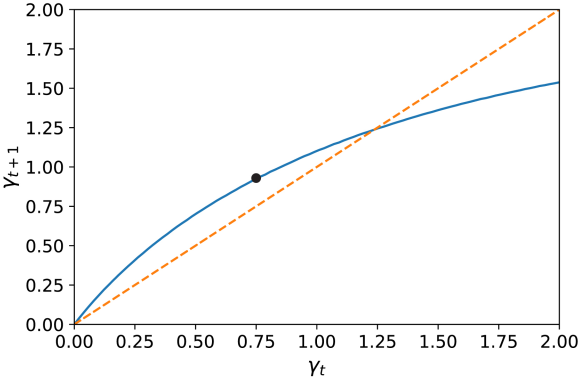
# Fixed points of state evolution




- If $\mathbb{E}\langle \boldsymbol{x}^0, \boldsymbol{v} \rangle = 0$, then $\gamma_t = 0$ is an (unstable) fixed point.
- This is the case in problems where $\boldsymbol{v}$ has zero mean, as $\boldsymbol{x}^0$ is independent of $\boldsymbol{v}$

# Spectral Initialization

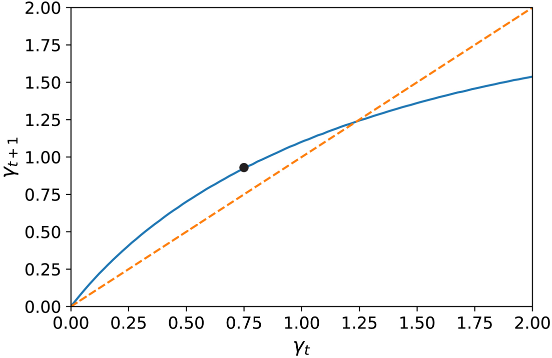
$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^\mathsf{T} + \boldsymbol{W}, \qquad \lambda > 1$$




- Compute $\varphi_1$, the principal eigenvector of $\boldsymbol{A}$
- Run AMP with initialization $\boldsymbol{x}^0 = \sqrt{n}\varphi_1$
- $\gamma_0 > 0$ as $\frac{1}{n}|\mathbb{E}\langle \boldsymbol{x}^0, \boldsymbol{v}\rangle| \to \sqrt{1-\lambda^{-2}}$

# AMP with spectral initialization

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$




$$\boldsymbol{x}^{t+1} = \boldsymbol{A}\, f_t(\boldsymbol{x}^t) \,-\, \mathsf{b}_t f_{t-1}(\boldsymbol{x}^{t-1}), \qquad \boldsymbol{x}^0 = \sqrt{n}\boldsymbol{\varphi}_1$$

Existing AMP analysis does not apply for initialization $\boldsymbol{x}^0$ *correlated* with $\boldsymbol{v}$

# AMP analysis with spectral initialization

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

Let $(\varphi_1, z_1)$ are the principal eigenvector and eigenvalue of $\boldsymbol{A}$

Instead of $\boldsymbol{A}$, we will analyze AMP on

$$\tilde{\boldsymbol{A}} = z_1\varphi_1\varphi_1^{\mathsf{T}} + \boldsymbol{P}^{\perp}\left(\frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \tilde{\boldsymbol{W}}\right)\boldsymbol{P}^{\perp}$$

- $\boldsymbol{P}^{\perp} = \boldsymbol{I} - \varphi_1\varphi_1^{\mathsf{T}}$
- $\tilde{\boldsymbol{W}} \sim \mathrm{GOE}(n)$ is independent of $\boldsymbol{W}$

# True vs conditional model

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

$$\tilde{\boldsymbol{A}} = z_1\,\boldsymbol{\varphi}_1\boldsymbol{\varphi}_1^{\mathsf{T}} + \boldsymbol{P}^{\perp}\left(\frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \tilde{\boldsymbol{W}}\right)\boldsymbol{P}^{\perp}$$

**Lemma**

For $(z_1, \boldsymbol{\varphi}_1) \in \left\{ |z_1 - (\lambda + \lambda^{-1})| \leq \varepsilon, \quad (\boldsymbol{\varphi}_1^{\mathsf{T}}\boldsymbol{v})^2 \geq 1 - \lambda^{-2} - \varepsilon \right\}$,

we have

$$\sup_{(\boldsymbol{z}_{\hat{S}}, \boldsymbol{\Phi}_{\hat{S}}) \in \mathcal{E}_\varepsilon} \left\| \mathbb{P}\left(\boldsymbol{A} \in \cdot \,\middle|\, z_1, \boldsymbol{\varphi}_1\right) - \mathbb{P}\left(\tilde{\boldsymbol{A}} \in \cdot \,\middle|\, z_1, \boldsymbol{\varphi}_1\right) \right\|_{\mathrm{TV}} \leq \frac{1}{c(\varepsilon)}\, e^{-nc(\varepsilon)}$$

# AMP on conditional model

$$\tilde{\boldsymbol{A}} = z_1 \varphi_1 \varphi_1^\mathsf{T} + \boldsymbol{P}^\perp \left( \frac{\lambda}{n} \boldsymbol{v}\boldsymbol{v}^\mathsf{T} + \tilde{\boldsymbol{W}} \right) \boldsymbol{P}^\perp$$

AMP with $\tilde{\boldsymbol{A}}$ instead of $\boldsymbol{A}$:

$$\tilde{\boldsymbol{x}}^{t+1} = \tilde{\boldsymbol{A}} f(\tilde{\boldsymbol{x}}^t; t) - \mathrm{b}_t f(\tilde{\boldsymbol{x}}^{t-1}; t-1), \qquad \tilde{\boldsymbol{x}}^0 = \sqrt{n}\,\varphi_1$$

Analyze using existing AMP analysis + results from random matrix theory

# Model assumptions

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

Let $\boldsymbol{v} = \boldsymbol{v}(n) \in \mathbb{R}^n$ be a sequence such that the empirical distribution of entries of $\boldsymbol{v}(n)$ converges weakly to $P_V$,

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Performance of any estimator $\hat{\boldsymbol{v}}$ measured via loss function $\psi : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$:

$$\psi(\boldsymbol{v}, \hat{\boldsymbol{v}}) = \frac{1}{n}\sum_{i=1}^{n} \psi(v_i, \hat{v}_i).$$

$\psi$ assumed to be *pseudo-Lipschitz*:

$$|\psi(\boldsymbol{x}) - \psi(\boldsymbol{y})| \le C\|\boldsymbol{x} - \boldsymbol{y}\|_2 \,(1 + \|\boldsymbol{x}\|_2 + \|\boldsymbol{y}\|_2), \qquad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^2$$

# Result for rank one case

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

Theorem: Let $\lambda > 1$. Consider the AMP

$$\boldsymbol{x}^{t+1} = \boldsymbol{A}\, f_t(\boldsymbol{x}^t) \,-\, \mathrm{b}_t f_{t-1}(\boldsymbol{x}^{t-1})$$

- Assume $f_t : \mathbb{R} \to \mathbb{R}$ is Lipschitz continuous
- Initialize with $\boldsymbol{x}^0 = \sqrt{n}\boldsymbol{\varphi}_1$

Then for any pseudo-Lipschitz loss function $\psi$ and $t \geq 0$,

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} \psi(v_i, x_i^t) = \mathbb{E}\left\{\psi(V, \mu_t V + \sigma_t G)\right\} \quad \text{a.s.}$$

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The state evolution parameters are recursively defined as

$$\mu_{t+1} = \lambda\,\mathbb{E}[V\, f_t(\mu_t V + \sigma_t G)], \quad \sigma_{t+1}^2 = \mathbb{E}[f_t(\mu_t V + \sigma_t G)^2],$$

# Bayes-optimal AMP

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

$$\boldsymbol{x}^{t+1} = \boldsymbol{A}\, f_t(\boldsymbol{x}^t) \; - \; \mathrm{b}_t f_{t-1}(\boldsymbol{x}^{t-1})$$

- Bayes-optimal choice $f_t(y) = \lambda\,\mathbb{E}(V \mid \gamma_t\, V + \sqrt{\gamma_t}\, G = y)$
- State evolution:

$$\gamma_{t+1} = \lambda^2\{1 - \mathrm{mmse}(\gamma_t)\}, \qquad \gamma_0 = \lambda^2 - 1$$

where $\mathrm{mmse}(\gamma) = \mathbb{E}\{\,[V - \mathbb{E}(V \mid \sqrt{\gamma}\, V + G)]^2\}$

- $\mu_t = \sigma_t^2 = \gamma_t$

# Bayes-optimal AMP

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

Let $\gamma_{\rm AMP}(\lambda)$ be the *smallest* strictly positive solution of

$$\gamma = \lambda^2[1 - \mathrm{mmse}(\gamma)]. \quad (1)$$

Then the AMP estimate $\hat{\boldsymbol{x}}^t = f_t(\boldsymbol{x}^t)$ achieves

$$\lim_{t\to\infty} \lim_{n\to\infty} \min_{s\in\{+1,-1\}} \frac{1}{n}\|\hat{\boldsymbol{x}}^t - s\boldsymbol{v}\|_2^2 = 1 - \frac{\gamma_{\rm AMP}(\lambda)}{\lambda^2}$$

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$$\text{Overlap}: \quad \lim_{t\to\infty}\lim_{n\to\infty} \frac{|\langle \hat{\boldsymbol{x}}^t, \boldsymbol{v}\rangle|}{\|\hat{\boldsymbol{x}}^t\|_2\|\boldsymbol{v}\|_2} = \frac{\sqrt{\gamma_{\mathrm{AMP}}(\lambda)}}{\lambda}$$

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### Bayes-optimal overlap [Miolane-Lelarge '16]

For (almost) all $\lambda > 0$

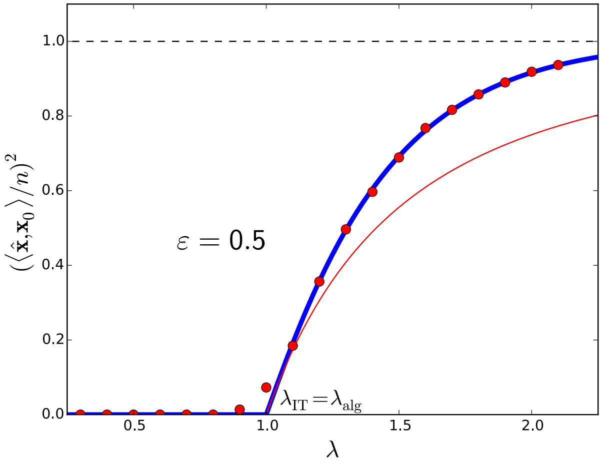
$$\lim_{n\to\infty}\sup_{\hat{\boldsymbol{x}}(\,\cdot\,)} \frac{|\langle \hat{\boldsymbol{x}}^t, \boldsymbol{v}\rangle|}{\|\hat{\boldsymbol{x}}^t\|_2\|\boldsymbol{v}\|_2} = \frac{\sqrt{\gamma_{\rm Bayes}(\lambda)}}{\lambda}$$

$\gamma_{\rm Bayes}(\lambda)$ is fixed point of (1) that maximizes a specified free-energy functional

# Example: Two-point mixture

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{v}\boldsymbol{v}^{\mathsf{T}} + \boldsymbol{W}$$

$$P_V = \varepsilon\,\delta_{a_+} + (1-\varepsilon)\delta_{a_-} \qquad a_+ = \sqrt{\frac{1-\varepsilon}{\varepsilon}} \quad a_- = -\sqrt{\frac{\varepsilon}{1-\varepsilon}}\,.$$



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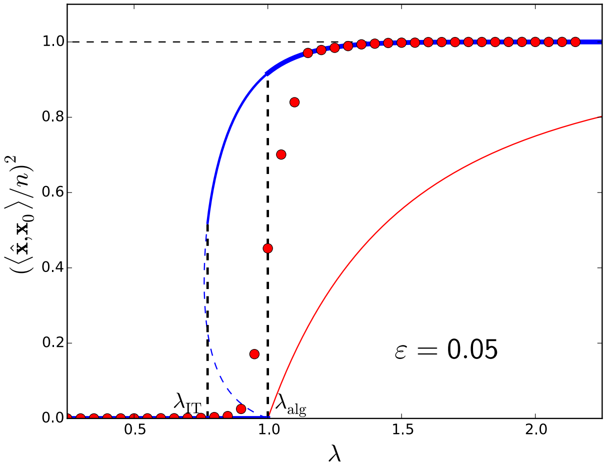

# General case

$$\boldsymbol{A} = \sum_{i=1}^{k} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^{\mathsf{T}} + \boldsymbol{W} \equiv \boldsymbol{V} \boldsymbol{\Lambda} \boldsymbol{V}^{\mathsf{T}} + \boldsymbol{W} \, .$$

- Assume $k_*$ eigenvectors corresponding to outliers $|\lambda_i| > 1$
- Outliers can be estimated from $\boldsymbol{A}$, as $z_i \to \lambda_i + \lambda_i^{-1}$
- Assume each row of $\boldsymbol{V} \sim P_{\boldsymbol{V}}$

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$$\text{AMP}: \qquad \boldsymbol{x}^{t+1} = \boldsymbol{A} f_t(\boldsymbol{x}^t) - f_{t-1}(\boldsymbol{x}^{t-1})\, \mathrm{B}_t^{\mathsf{T}}$$

- $\boldsymbol{x}^t \in \mathbb{R}^{n \times k_*}$ are estimates of the outlier eigenvectors
- $f(\cdot\,; t) : \mathbb{R}^{k_*} \to \mathbb{R}^{k_*}$ applied row by row
- $\mathrm{B}_t = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial f_t}{\partial \boldsymbol{x}}(\boldsymbol{x}_i^t)$, where $\frac{\partial f_t}{\partial \boldsymbol{x}}$ is Jacobian of $f(\cdot\,; t)$

Spectral initialization: $\boldsymbol{x}^0 = \left[\sqrt{n}\varphi_1 \mid \ldots \mid \sqrt{n}\varphi_{k_*}\right]$

# Example: Gaussian block model

Let $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_n)$ be vector of vertex labels

Labels $\sigma_i$ uniformly distributed in $\{1, 2, 3\}$

Consider the $n \times n$ matrix $\boldsymbol{A}_0$ with entries

$$A_{0,ij} = \begin{cases} 2/n & \text{if } \sigma_i = \sigma_j \\ -1/n & \text{otherwise.} \end{cases}$$

$\boldsymbol{A}_0$ is an orthogonal projector onto a two-dimensional subspace

Wish to estimate $\boldsymbol{A}_0$ from noisy version:

$$\boldsymbol{A} = \lambda \boldsymbol{A}_0 + \boldsymbol{W}$$

Degenerate eigenvalues: $\lambda_1 = \lambda_2 = \lambda$

# AMP

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{V}\boldsymbol{V}^{\mathsf{T}} + \boldsymbol{W}$$

Spectral initialization: $\boldsymbol{x}^0 = [\sqrt{n}\varphi_1 \quad \sqrt{n}\varphi_2]$

## Main result

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} \psi(\boldsymbol{x}_i^t, \boldsymbol{V}_i) = \mathbb{E}\{\psi(\boldsymbol{M}_t \underline{V} + \boldsymbol{Q}_t^{1/2}\underline{G}, \underline{V})\} \quad \text{a.s.}$$

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State evolution: $\boldsymbol{M}_0 = (\boldsymbol{x}^0)^{\mathsf{T}}\boldsymbol{V} \in \mathbb{R}^{2\times 2}$ and

$$\boldsymbol{M}_{t+1} = \lambda\mathbb{E}\Big\{f_t(\boldsymbol{M}_t\underline{V} + \boldsymbol{Q}_t^{1/2}\underline{G})\underline{V}^{\mathsf{T}}\Big\},$$

$$\boldsymbol{Q}_{t+1} = \mathbb{E}\Big\{f_t(\boldsymbol{M}_t\underline{V} + \boldsymbol{Q}_t^{1/2}\boldsymbol{G})f_t(\boldsymbol{M}_t\underline{V} + \boldsymbol{Q}_t^{1/2}\underline{G})^{\mathsf{T}}\Big\}.$$

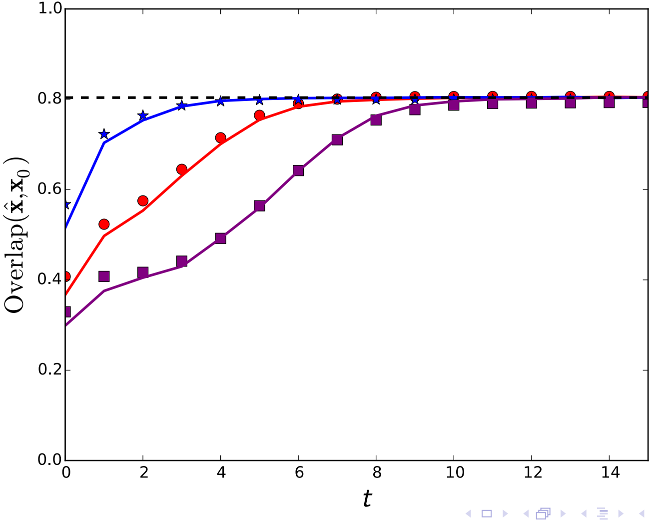
Since $\boldsymbol{V}\boldsymbol{V}^{\mathsf{T}} = \boldsymbol{V}\boldsymbol{R}\boldsymbol{R}^{\mathsf{T}}\boldsymbol{V}^{\mathsf{T}}$ for any $2\times 2$ rotation matrix $\boldsymbol{R}$

$\Rightarrow$ state evolution starts from a *random* initial condition

$$\boldsymbol{M}_0 = (\boldsymbol{x}^0)^{\mathsf{T}}\boldsymbol{V} \stackrel{d}{=} \sqrt{1-\lambda^{-2}}\boldsymbol{R}$$

$$\boldsymbol{A} = \frac{\lambda}{n}\boldsymbol{U}\boldsymbol{U}^{\mathsf{T}} + \boldsymbol{W}$$

Gaussian block model with $\lambda = 1.5$, $n = 6000$



# Summary

$$\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{\mathsf{T}} + \boldsymbol{W}$$

AMP with spectral initialization

- Distributional property of the iterates gives succinct performance characterization via state evolution
- Can be used to construct confidence intervals
- AMP can achieve Bayes-optimal accuracy

**Extensions and Future work**

- Can be extended to rectangular low-rank matrix model: $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^{\mathsf{T}} + \boldsymbol{W}$
- Spectral initialization for other problems, e.g., phase retrieval

`https://arxiv.org/abs/1711.01682`