

Low-rank Matrix Estimation via Approximate Message Passing

Ramji Venkataramanan

Department of Engineering

(Joint work with Andrea Montanari)

October 31, 2018

CCIMI Seminar

Symmetric Low-rank Model

$$\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{v}_i \mathbf{v}_i^T + \mathbf{W} \quad \in \mathbb{R}^{n \times n}$$

- ▶ $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$ are deterministic scalars
- ▶ $\mathbf{v}_1, \dots, \mathbf{v}_k \in \mathbb{R}^n$ are orthonormal vectors (“spikes”)
- ▶ \mathbf{W} is a symmetric noise matrix

GOAL: To estimate the vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ from \mathbf{A}

Rectangular Low-rank model

$$\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{u}_i \mathbf{v}_i^T + \mathbf{W} \quad \in \mathbb{R}^{m \times n}$$

- ▶ $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$ are deterministic scalars
- ▶ $\mathbf{u}_1, \dots, \mathbf{u}_k \in \mathbb{R}^m$ are left singular vectors
 $\mathbf{v}_1, \dots, \mathbf{v}_k \in \mathbb{R}^n$ are right singular vectors
- ▶ \mathbf{W} is a noise matrix

GOAL: Estimate the singular vectors $\mathbf{u}_1, \dots, \mathbf{u}_k$ and $\mathbf{v}_1, \dots, \mathbf{v}_k$

Applications

$$\begin{bmatrix} & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \end{bmatrix} \mathbf{A} \approx \begin{bmatrix} & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \end{bmatrix} \mathbf{U} \begin{bmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} \mathbf{V}^T$$

$n \times d$ $n \times k$ $k \times d$

Topic Modelling

- ▶ Each row of \mathbf{A} is a document
- ▶ Each row of \mathbf{V}^T is a topic
- ▶ Each document convex combination of k topics

Hidden clique

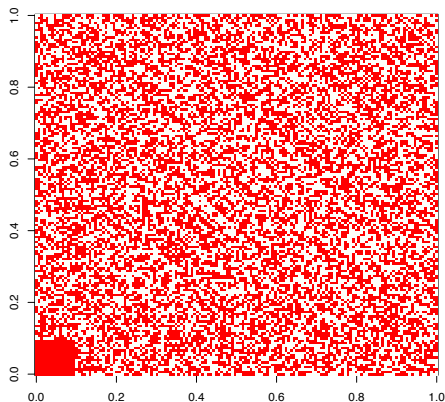


Image from *Statistical Estimation: From Denoising to Sparse Regression and Hidden Cliques* by A. Montanari

Hidden clique

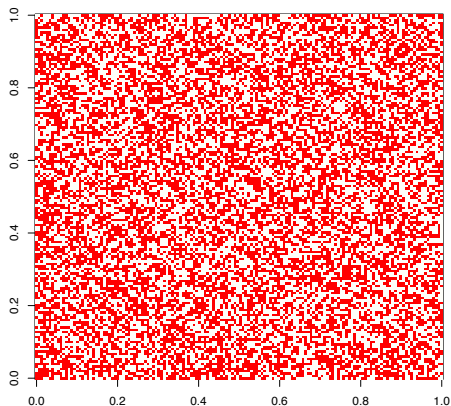


Image from *Statistical Estimation: From Denoising to Sparse Regression and Hidden Cliques* by A. Montanari

Hidden clique

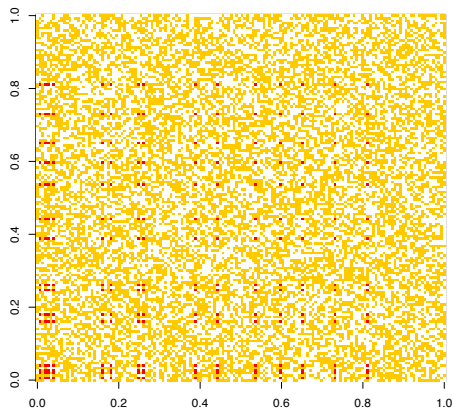
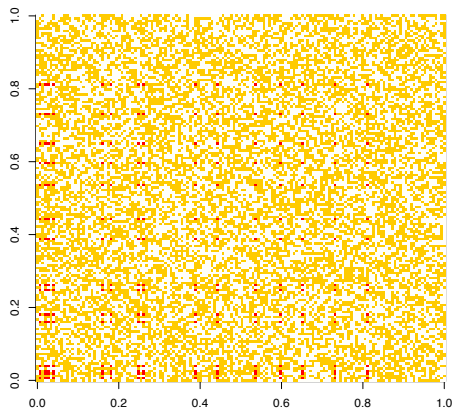


Image from *Statistical Estimation: From Denoising to Sparse Regression and Hidden Cliques* by A. Montanari

Hidden clique



For hidden clique S , adjacency matrix has the form

$$\mathbf{A} = \mathbf{1}_S \mathbf{1}_S^T + \mathbf{W}$$

Symmetric Spiked Model

$$\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{v}_i \mathbf{v}_i^T + \mathbf{W} \quad \in \mathbb{R}^{n \times n}$$

- ▶ $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$ are deterministic scalars
- ▶ $\mathbf{v}_1, \dots, \mathbf{v}_k \in \mathbb{R}^n$ are orthonormal vectors (“spikes”)
- ▶ $\mathbf{W} \sim \text{GOE}(n) \Rightarrow \mathbf{W}$ symmetric with
 $(W_{ii})_{i \leq n} \sim i.i.d. \text{N}(0, \frac{2}{n})$ and $(W_{ij})_{i < j \leq n} \sim i.i.d. \text{N}(0, \frac{1}{n})$

Spectrum of spiked matrix

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

Random matrix theory and the 'BBAP' phase transition :

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

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

- ▶ Eigenvectors φ_i corresponding to outliers z_i satisfy

$$|\langle \varphi_i, \mathbf{v}_i \rangle| \rightarrow \sqrt{1 - \frac{1}{\lambda_i^2}}$$

Structural information

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

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

- ▶ Best estimator of \mathbf{v}_i is the i th eigenvector φ_i
- ▶ If $|\lambda_i| \geq 1$, then $|\langle \mathbf{v}_i, \varphi_i \rangle| \rightarrow \sqrt{1 - \frac{1}{\lambda_i^2}}$

Structural information

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

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

- ▶ Best estimator of \mathbf{v}_i is the i th eigenvector φ_i
- ▶ If $|\lambda_i| \geq 1$, then $|\langle \mathbf{v}_i, \varphi_i \rangle| \rightarrow \sqrt{1 - \frac{1}{\lambda_i^2}}$

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

- ▶ For example, \mathbf{v}_i 's may be sparse, bounded, non-negative etc.
- ▶ Relevant in sparse PCA, non-negative PCA, hidden clique, community detection under stochastic block model, ...
- ▶ Can improve on spectral methods

Prior on eigenvectors

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

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

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

$$\hat{\mathbf{V}}_{\text{Bayes}} = \mathbb{E}[\mathbf{V} \mid \mathbf{A}]$$

- ▶ Generally not computable
- ▶ Closed-form expressions for asymptotic Bayes risk

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

Computable estimators

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

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

Computable estimators

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

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

In this talk

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

Rank one spiked model

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

Power iteration for principal eigenvector:

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

Rank one spiked model

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

Power iteration for principal eigenvector:

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

AMP:

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

- ▶ Non-linear function $f_t : \mathbb{R} \rightarrow \mathbb{R}$ chosen based on structural info on \mathbf{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

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

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

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

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

State evolution

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

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

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

- ▶ $\mathbf{g} \sim_{i.i.d.} \mathcal{N}(0, 1)$, independent of $\mathbf{v} \sim_{i.i.d.} P_V$
- ▶ Scalars μ_t, σ_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 $\mu_0 = \frac{1}{n} |\mathbb{E}\langle \mathbf{x}^0, \mathbf{v} \rangle|$, $\sigma_0^2 = \mathbb{E}V^2 - \mu_0^2$

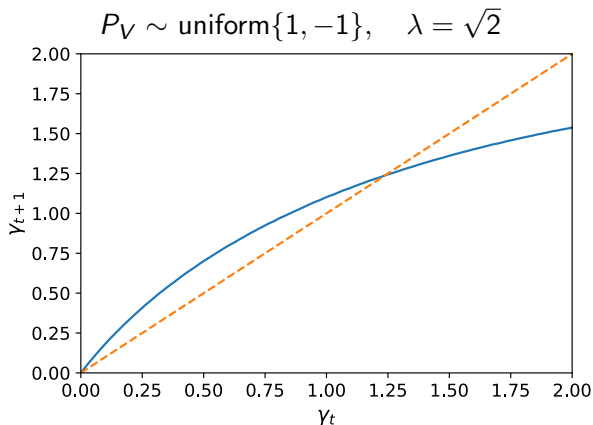
Bayes-optimal AMP

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

Bayes-optimal AMP

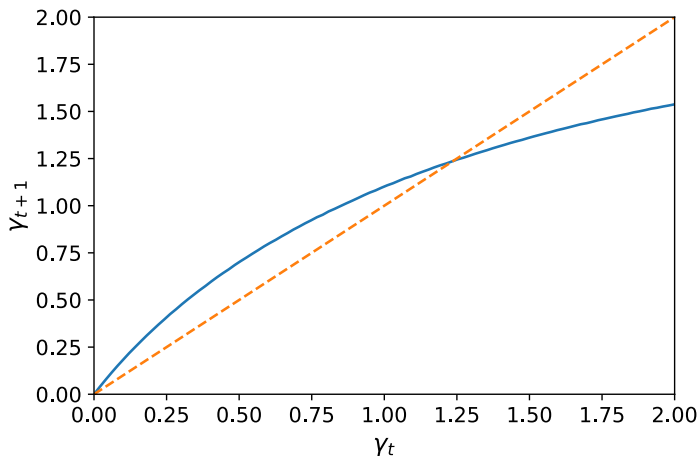
Assuming $\mathbf{x}^t = \mu_t \mathbf{v} + \sigma_t \mathbf{g}$, choose $f_t(y) = \lambda \mathbb{E}[V \mid \mu_t V + \sigma_t G = y]$

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



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

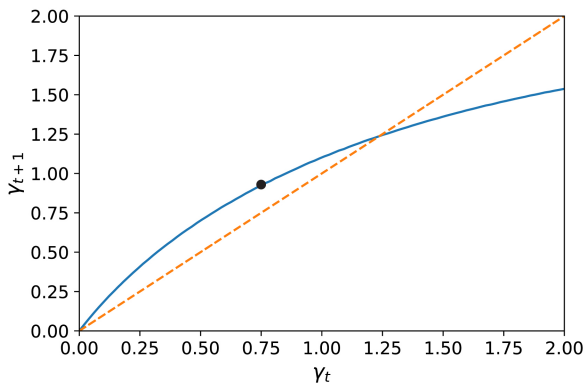
Fixed points of state evolution



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

Spectral Initialization

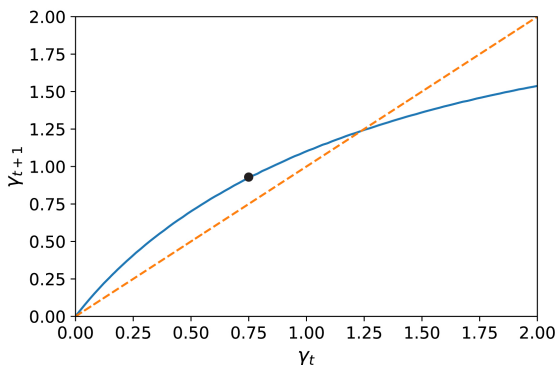
$$\mathbf{A} = \frac{\lambda}{n} \mathbf{v} \mathbf{v}^T + \mathbf{W}, \quad \lambda > 1$$



- ▶ Compute φ_1 , the principal eigenvector of \mathbf{A}
- ▶ Run AMP with initialization $\mathbf{x}^0 = \sqrt{n} \varphi_1$
- ▶ $\gamma_0 > 0$ as $\frac{1}{n} |\mathbb{E} \langle \mathbf{x}^0, \mathbf{v} \rangle| \rightarrow \sqrt{1 - \lambda^{-2}}$

AMP with spectral initialization

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



$$\mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1}), \quad \mathbf{x}^0 = \sqrt{n} \varphi_1$$

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

Standard AMP analysis

With $\mathbf{W} \sim \text{GOE}(n)$, consider

$$\mathbf{h}^{t+1} = \mathbf{W} f_t(\mathbf{h}^t) - b_t f_{t-1}(\mathbf{h}^{t-1})$$

Initialised with \mathbf{h}^0 independent of \mathbf{W} . Let $\vartheta_t := \{\mathbf{h}^0, \dots, \mathbf{h}^t\}$

Standard AMP analysis

With $\mathbf{W} \sim \text{GOE}(n)$, consider

$$\mathbf{h}^{t+1} = \mathbf{W} f_t(\mathbf{h}^t) - b_t f_{t-1}(\mathbf{h}^{t-1})$$

Initialised with \mathbf{h}^0 independent of \mathbf{W} . Let $\vartheta_t := \{\mathbf{h}^0, \dots, \mathbf{h}^t\}$

- ▶ Conditional distribution

$$\mathbf{W}|_{\vartheta_t} \stackrel{d}{=} \mathbb{E}[\mathbf{W} | \vartheta_t] + \mathbf{P}_{\vartheta_t}^{\perp} \tilde{\mathbf{W}} \mathbf{P}_{\vartheta_t}^{\perp}$$

Standard AMP analysis

With $\mathbf{W} \sim \text{GOE}(n)$, consider

$$\mathbf{h}^{t+1} = \mathbf{W} f_t(\mathbf{h}^t) - b_t f_{t-1}(\mathbf{h}^{t-1})$$

Initialised with \mathbf{h}^0 independent of \mathbf{W} . Let $\vartheta_t := \{\mathbf{h}^0, \dots, \mathbf{h}^t\}$

- ▶ Conditional distribution

$$\mathbf{W}|_{\vartheta_t} \stackrel{d}{=} \mathbb{E}[\mathbf{W} | \vartheta_t] + \mathbf{P}_{\vartheta_t}^{\perp} \tilde{\mathbf{W}} \mathbf{P}_{\vartheta_t}^{\perp}$$

- ▶ By induction, show that for $t \geq 0$:

$$\mathbf{h}^{t+1} = \sum_{i=0}^t \alpha_i \mathbf{h}^i + \mathbf{g}_t + \mathbf{\Delta}_t$$

Standard AMP analysis

With $\mathbf{W} \sim \text{GOE}(n)$, consider

$$\mathbf{h}^{t+1} = \mathbf{W} f_t(\mathbf{h}^t) - b_t f_{t-1}(\mathbf{h}^{t-1})$$

Initialised with \mathbf{h}^0 independent of \mathbf{W} . Let $\vartheta_t := \{\mathbf{h}^0, \dots, \mathbf{h}^t\}$

- ▶ Conditional distribution

$$\mathbf{W}|_{\vartheta_t} \stackrel{d}{=} \mathbb{E}[\mathbf{W} | \vartheta_t] + \mathbf{P}_{\vartheta_t}^{\perp} \tilde{\mathbf{W}} \mathbf{P}_{\vartheta_t}^{\perp}$$

- ▶ By induction, show that for $t \geq 0$:

$$\mathbf{h}^{t+1} = \sum_{i=0}^t \alpha_i \mathbf{h}^i + \mathbf{g}_t + \mathbf{\Delta}_t$$

$$\mathbf{h}^{t+1} \stackrel{d}{\approx} \tau_t \mathbf{g} \quad \tau_t^2 = \mathbb{E}[f_t(\tau_{t-1} G)^2], \quad \tau_0^2 = \|f(\mathbf{h}^0)\|^2/n$$

AMP with spectral initialization

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

Let (φ_1, z_1) be principal eigenvector and eigenvalue of \mathbf{A}

$$\mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1})$$

initialised with $\mathbf{x}^0 = \sqrt{n} \varphi_1$

AMP with spectral initialization

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

Let (φ_1, z_1) be principal eigenvector and eigenvalue of \mathbf{A}

$$\mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1})$$

initialised with $\mathbf{x}^0 = \sqrt{n} \varphi_1$

We write

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

► $\mathbf{P}^\perp = \mathbf{I} - \varphi_1 \varphi_1^T$

AMP with spectral initialization

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

Let (φ_1, z_1) be principal eigenvector and eigenvalue of \mathbf{A}

$$\mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1})$$

initialised with $\mathbf{x}^0 = \sqrt{n} \varphi_1$

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

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

- ▶ $\mathbf{P}^\perp = \mathbf{I} - \varphi_1 \varphi_1^T$
 - ▶ $\tilde{\mathbf{W}} \sim \text{GOE}(n)$ is independent of \mathbf{W}
1. Conditioned on z_1 and $(\varphi_1^T \mathbf{v})^2$ being close to limiting values, total variation distance between \mathbf{A} and $\tilde{\mathbf{A}}$ is small

AMP with spectral initialization

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

Let (φ_1, z_1) be principal eigenvector and eigenvalue of \mathbf{A}

$$\mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1})$$

initialised with $\mathbf{x}^0 = \sqrt{n} \varphi_1$

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

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

- ▶ $\mathbf{P}^\perp = \mathbf{I} - \varphi_1 \varphi_1^T$
 - ▶ $\tilde{\mathbf{W}} \sim \text{GOE}(n)$ is independent of \mathbf{W}
1. Conditioned on z_1 and $(\varphi_1^T \mathbf{v})^2$ being close to limiting values, total variation distance between \mathbf{A} and $\tilde{\mathbf{A}}$ is small
 2. Analyze AMP on $\tilde{\mathbf{A}}$ by extending standard AMP analysis

Model assumptions

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

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

Model assumptions

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

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

Performance of any estimator $\hat{\mathbf{v}}$ measured via loss function

$\psi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$:

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

ψ assumed to be *pseudo-Lipschitz*:

$$|\psi(\mathbf{x}) - \psi(\mathbf{y})| \leq C \|\mathbf{x} - \mathbf{y}\|_2 (1 + \|\mathbf{x}\|_2 + \|\mathbf{y}\|_2), \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^2$$

L_2 loss, L_1 loss are both pseudo-Lipschitz

Result for rank one case

$$\mathbf{A} = \frac{\lambda}{n} \mathbf{v} \mathbf{v}^\top + \mathbf{W}$$

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

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

- ▶ Assume $f_t : \mathbb{R} \rightarrow \mathbb{R}$ is Lipschitz continuous
- ▶ Initialize with $\mathbf{x}^0 = \sqrt{n} \varphi_1$

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

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

Result for rank one case

$$\mathbf{A} = \frac{\lambda}{n} \mathbf{v} \mathbf{v}^\top + \mathbf{W}$$

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

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

- ▶ Assume $f_t : \mathbb{R} \rightarrow \mathbb{R}$ is Lipschitz continuous
- ▶ Initialize with $\mathbf{x}^0 = \sqrt{n} \varphi_1$

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

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

State evolution parameters: $\mu_0 = \sqrt{1 - \lambda^{-2}}$, $\sigma_0 = 1/\lambda$,

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

Proof Sketch

True vs conditional model

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

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

Lemma

For $(z_1, \varphi_1) \in \left\{ |z_1 - (\lambda + \lambda^{-1})| \leq \varepsilon, \quad (\varphi_1^T \mathbf{v})^2 \geq 1 - \lambda^{-2} - \varepsilon \right\}$,

we have

$$\sup_{(z_{\hat{S}}, \Phi_{\hat{S}}) \in \mathcal{E}_\varepsilon} \left\| \mathbb{P}(\mathbf{A} \in \cdot | z_1, \varphi_1) - \mathbb{P}(\tilde{\mathbf{A}} \in \cdot | z_1, \varphi_1) \right\|_{\text{TV}} \leq \frac{1}{c(\varepsilon)} e^{-nc(\varepsilon)}$$

AMP on conditional model

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

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

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

Analyze using existing AMP analysis + results from random matrix theory

Bayes-optimal AMP

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

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

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

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

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

- ▶ $\mu_t = \sigma_t^2 = \gamma_t$

Bayes-optimal AMP

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

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

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

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

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

Bayes-optimal AMP

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

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

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

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

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

Bayes-optimal AMP

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

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

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

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

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

Bayes-optimal overlap [Miolane-Lelarge '16]

For (almost) all $\lambda > 0$

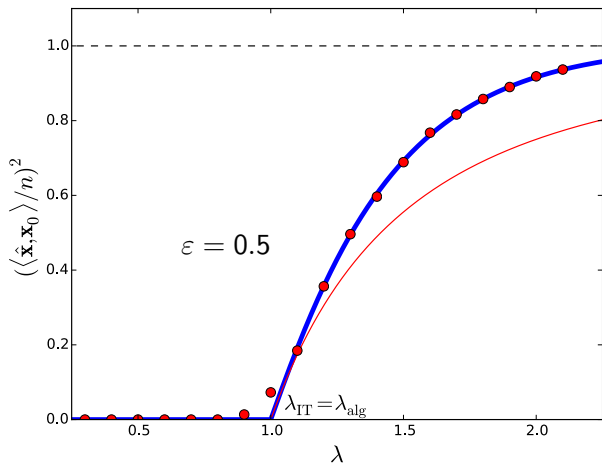
$$\lim_{n \rightarrow \infty} \sup_{\hat{\mathbf{x}}(\cdot)} \frac{|\langle \hat{\mathbf{x}}^t, \mathbf{v} \rangle|}{\|\hat{\mathbf{x}}^t\|_2 \|\mathbf{v}\|_2} = \frac{\sqrt{\gamma_{\text{Bayes}}(\lambda)}}{\lambda}$$

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

Example: Two-point mixture

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

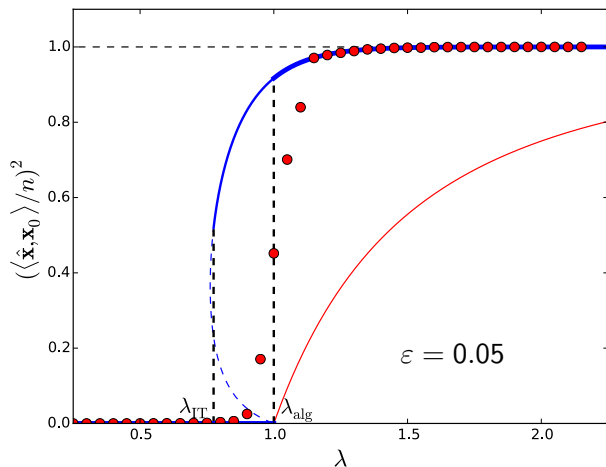
$$P_V = \varepsilon \delta_{a_+} + (1 - \varepsilon) \delta_{a_-} \quad a_+ = \sqrt{\frac{1 - \varepsilon}{\varepsilon}} \quad a_- = -\sqrt{\frac{\varepsilon}{1 - \varepsilon}}.$$



Example: Two-point mixture

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

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



Confidence intervals

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

$$\text{AMP: } \mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1})$$

- ▶ Convergence result tells us that $\mathbf{x}^t \approx \mu_t \mathbf{v} + \sigma_t \mathbf{g}$

Confidence intervals

$$\mathbf{A} = \frac{\lambda}{n} \mathbf{v} \mathbf{v}^\top + \mathbf{W}$$

$$\text{AMP: } \mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - \mathbf{b}_t f_{t-1}(\mathbf{x}^{t-1})$$

- ▶ Convergence result tells us that $\mathbf{x}^t \approx \mu_t \mathbf{v} + \sigma_t \mathbf{g}$
- ▶ State evolution parameters can be estimated:

$$\hat{\sigma}_t^2 \equiv \frac{1}{n} \|f_{t-1}(\mathbf{x}^{t-1})\|_2^2,$$

$$\hat{\mu}_t^2 \equiv \frac{1}{n} \|\mathbf{x}^t\|_2^2 - \frac{1}{n} \|f_{t-1}(\mathbf{x}^{t-1})\|_2^2.$$

Confidence intervals

$$\mathbf{A} = \frac{\lambda}{n} \mathbf{v} \mathbf{v}^\top + \mathbf{W}$$

$$\text{AMP: } \mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - b_t f_{t-1}(\mathbf{x}^{t-1})$$

- ▶ Convergence result tells us that $\mathbf{x}^t \approx \mu_t \mathbf{v} + \sigma_t \mathbf{g}$
- ▶ State evolution parameters can be estimated:

$$\hat{\sigma}_t^2 \equiv \frac{1}{n} \|f_{t-1}(\mathbf{x}^{t-1})\|_2^2,$$

$$\hat{\mu}_t^2 \equiv \frac{1}{n} \|\mathbf{x}^t\|_2^2 - \frac{1}{n} \|f_{t-1}(\mathbf{x}^{t-1})\|_2^2.$$

- ▶ Confidence intervals for coverage level $(1 - \alpha)$:

$$\hat{l}_i(\alpha; t) = \left[\frac{1}{\hat{\mu}_t} x_i^t - \frac{\hat{\sigma}_t}{\hat{\mu}_t} \Phi^{-1} \left(1 - \frac{\alpha}{2} \right), \frac{1}{\hat{\mu}_t} x_i^t + \frac{\hat{\sigma}_t}{\hat{\mu}_t} \Phi^{-1} \left(1 - \frac{\alpha}{2} \right) \right]$$

- ▶ Bayes-optimal choice minimizes length of confidence intervals, but requires knowledge of the empirical distribution of \mathbf{v}

For $1 \leq i \leq n$,

$$\hat{l}_i(\alpha; t) = \left[\frac{1}{\hat{\mu}_t} x_i^t - \frac{\hat{\sigma}_t}{\hat{\mu}_t} \Phi^{-1} \left(1 - \frac{\alpha}{2} \right), \frac{1}{\hat{\mu}_t} x_i^t + \frac{\hat{\sigma}_t}{\hat{\mu}_t} \Phi^{-1} \left(1 - \frac{\alpha}{2} \right) \right]$$

Corollary:

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \mathbb{I}(v_i \in \hat{l}_i(\alpha; t)) = 1 - \alpha \quad \text{almost surely.}$$

General case

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

- ▶ Assume k_* eigenvectors corresponding to outliers $|\lambda_i| > 1$
- ▶ Outliers can be estimated from \mathbf{A} , as $z_i \rightarrow \lambda_i + \lambda_i^{-1}$
- ▶ Assume empirical distribution of rows of $\mathbf{V} \sim P_{\mathbf{V}}$

General case

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

- ▶ Assume k_* eigenvectors corresponding to outliers $|\lambda_i| > 1$
- ▶ Outliers can be estimated from \mathbf{A} , as $z_i \rightarrow \lambda_i + \lambda_i^{-1}$
- ▶ Assume empirical distribution of rows of $\mathbf{V} \sim P_{\mathbf{V}}$

General case

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

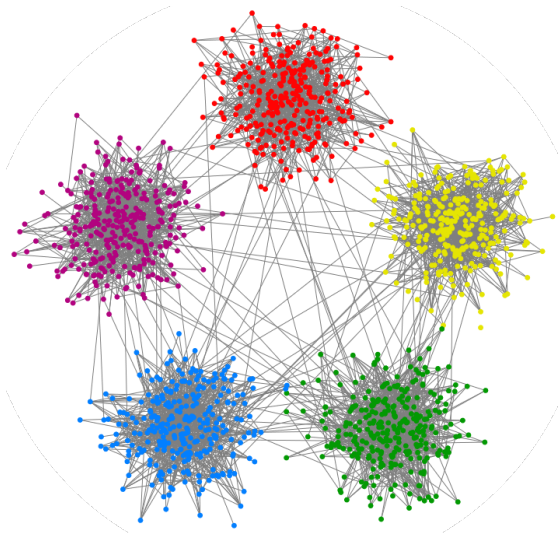
- ▶ Assume k_* eigenvectors corresponding to outliers $|\lambda_i| > 1$
- ▶ Outliers can be estimated from \mathbf{A} , as $z_i \rightarrow \lambda_i + \lambda_i^{-1}$
- ▶ Assume empirical distribution of rows of $\mathbf{V} \sim P_{\mathbf{V}}$

$$\text{AMP : } \quad \mathbf{x}^{t+1} = \mathbf{A} f_t(\mathbf{x}^t) - f_{t-1}(\mathbf{x}^{t-1}) \mathbf{B}_t^T$$

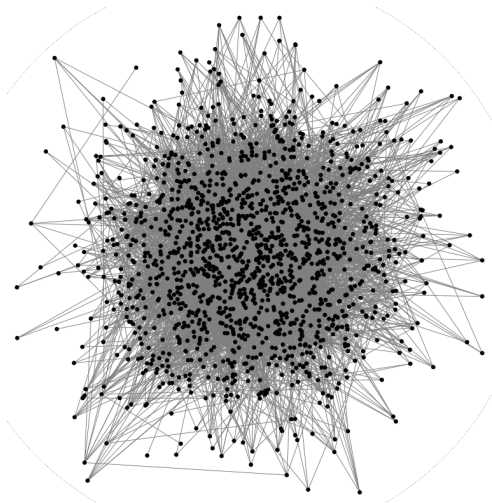
- ▶ $\mathbf{x}^t \in \mathbb{R}^{n \times k_*}$ are estimates of the outlier eigenvectors
- ▶ $f(\cdot; t) : \mathbb{R}^{k_*} \rightarrow \mathbb{R}^{k_*}$ applied row by row
- ▶ $\mathbf{B}_t = \frac{1}{n} \sum_{i=1}^n \frac{\partial f_t}{\partial \mathbf{x}}(\mathbf{x}_i^t)$, where $\frac{\partial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

Spectral initialization: $\mathbf{x}^0 = [\sqrt{n}\varphi_1 \mid \dots \mid \sqrt{n}\varphi_{k_*}]$

Block model with multiple communities



Block model with multiple communities



Wish to recover vertex labels (colours) from adjacency matrix

A closely related model ...

- ▶ Let $\sigma = (\sigma_1, \dots, \sigma_n)$ be vector of vertex labels
- ▶ Labels σ_i uniformly distributed in $\{1, 2, 3\}$
- ▶ Consider the $n \times n$ matrix \mathbf{A}_0 with entries

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

- ▶ \mathbf{A}_0 is an orthogonal projector onto a two-dimensional subspace $\Rightarrow \mathbf{A}_0$ is rank 2

A closely related model ...

- ▶ Let $\sigma = (\sigma_1, \dots, \sigma_n)$ be vector of vertex labels
- ▶ Labels σ_i uniformly distributed in $\{1, 2, 3\}$
- ▶ Consider the $n \times n$ matrix \mathbf{A}_0 with entries

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

- ▶ \mathbf{A}_0 is an orthogonal projector onto a two-dimensional subspace $\Rightarrow \mathbf{A}_0$ is rank 2

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

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

- ▶ Degenerate eigenvalues: $\lambda_1 = \lambda_2 = \lambda > 1$
- ▶ $\mathbf{W} \sim \text{GOE}(n)$
- ▶ \mathbf{A} similar to rescaled adjacency matrix in block model

AMP

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

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

Main result

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

AMP

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

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

Main result

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

State evolution: $\mathbf{M}_0 = (\mathbf{x}^0)^T \mathbf{V}$ and $\mathbf{Q}_0 = \lambda^{-1} \mathbf{I} \in \mathbb{R}^{2 \times 2}$

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

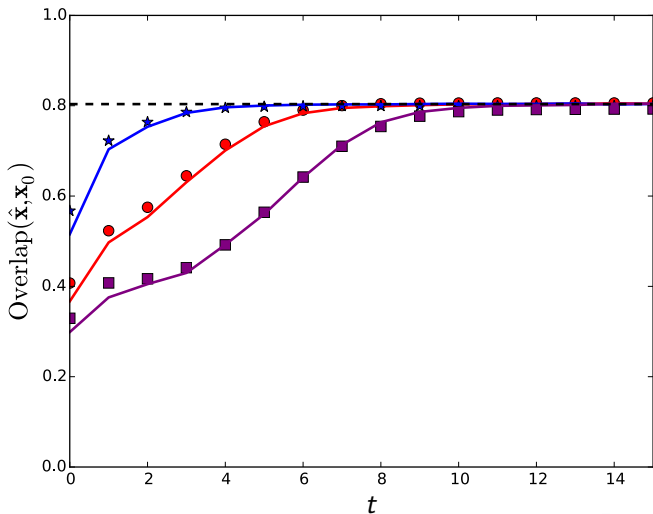
$$\mathbf{Q}_{t+1} = \mathbb{E}\left\{ f_t(\mathbf{M}_t \underline{V} + \mathbf{Q}_t^{1/2} \underline{G}) f_t(\mathbf{M}_t \underline{V} + \mathbf{Q}_t^{1/2} \underline{G})^T \right\}.$$

Since $\mathbf{V} \mathbf{V}^T = \mathbf{V} \mathbf{R} \mathbf{R}^T \mathbf{V}^T$ for any 2×2 rotation matrix \mathbf{R}
 \Rightarrow state evolution starts from a *random* initial condition

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

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

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



Summary

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

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:
$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T + \mathbf{W}$$
- ▶ AMP with spectral initialization for generalized linear models, e.g., phase retrieval

<https://arxiv.org/abs/1711.01682>