Statistical and Computational Tradeoffs in Biconvex Optimization

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Outline

- Motivations
- General theory of biconvex optimization
- Application 1: bigraphical model
- Application 2: joint clustering and network estimation
- Future work

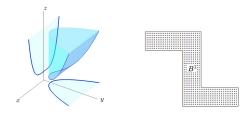
Background: Biconvex Optimization

- A function $g(x,y): \mathcal{A} \times \mathcal{B} \to \mathbb{R}$ is biconvex if g(x,y) is convex in x for fixed $y \in \mathcal{B}$, and convex in y for fixed $x \in \mathcal{A}$.
- Biconvex optimization:

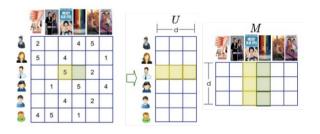
$$\min g(x,y)$$

$$s.t. x \in A, y \in B$$

Figure: Biconvex function and biconvex set



Motivation: Non-negative matrix factorization



Source: A. Karatzoglou, ESSIR 2013 Recommender Systems tutorial

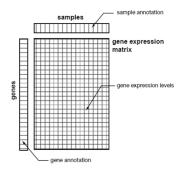
■ Non-negative matrix factorization solves

$$\min_{U,M} \ \frac{1}{2} \|X - UM\|_F^2$$
s.t. $U_{ij} \ge 0, M_{ij} \ge 0.$



Motivation: Bigraphical model

Traditional Graphical Model:



https://galton.uchicago.edu/ lafferty/research.html

Motivation: Bigraphical model

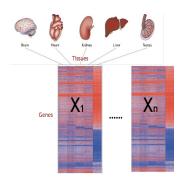


Figure : Matrix-variate data

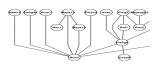


Figure : Gene network



Figure: Tissue network

Source: Yin and Li (2012)

Biconvex Optimization

■ Population objective function: $g(\mathbf{a}, \mathbf{b})$

$$(\mathbf{a}^*, \mathbf{b}^*) = \arg \min \ g(\mathbf{a}, \mathbf{b})$$

 $s.t. \ \mathbf{a} \in \mathcal{A}, \mathbf{b} \in \mathcal{B}$

- Sample objective function: $g_n(\mathbf{a}, \mathbf{b})$
- Goal: Find a minimizer $(\widehat{\mathbf{a}}, \widehat{\mathbf{b}})$ via $g_n(\mathbf{a}, \mathbf{b})$ s.t. $\|\widehat{\mathbf{a}} \mathbf{a}^*\|_2$ and $\|\widehat{\mathbf{b}} \mathbf{b}^*\|_2$ are small given limited computational resources.

Alternative Update Algorithm

Input: function $g_n(\mathbf{a}, \mathbf{b})$, maximal number of iterations T.

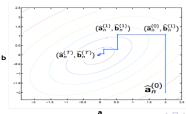
Initialize: $\widehat{\mathbf{a}}_n^{(0)}$

For t = 1 to T:

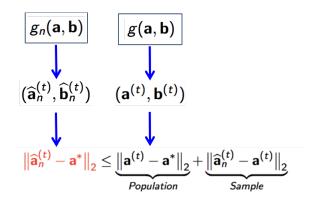
- Fix $\widehat{\mathbf{a}}_n^{(t-1)}$, update $\widehat{\mathbf{b}}_n^{(t)} = \arg\min_{\mathbf{b}} g_n(\widehat{\mathbf{a}}_n^{(t-1)}, \mathbf{b})$;
- Fix $\widehat{\mathbf{b}}_n^{(t)}$, update $\widehat{\mathbf{a}}_n^{(t)} = \arg\min_{\mathbf{a}} g_n(\mathbf{a}, \widehat{\mathbf{b}}_n^{(t)})$;

End For

Output: $\hat{\mathbf{a}} = \hat{\mathbf{a}}_n^{(T)}$ and $\hat{\mathbf{b}} = \hat{\mathbf{b}}_n^{(T)}$.



Theory: Outline



Theory: Population Version

• We focus on the Euclidean ball of radius $\alpha > 0$ for \mathcal{A} and \mathcal{B} .

$$\mathcal{A} = \mathcal{B}(\alpha; \mathbf{a}^*) := \{ \mathbf{a} \in \mathbb{R}^p : ||\mathbf{a} - \mathbf{a}^*||_2 \le \alpha \}$$

$$\mathcal{B} = \mathcal{B}(\alpha; \mathbf{b}^*) := \{ \mathbf{b} \in \mathbb{R}^q : ||\mathbf{b} - \mathbf{b}^*||_2 \le \alpha \}$$

■ Denote $\nabla_1 g(\mathbf{a}, \mathbf{b})$ be the gradient w.r.t. \mathbf{a} and $\nabla_2 g(\mathbf{a}, \mathbf{b})$ be the gradient w.r.t. \mathbf{b} .

Condition $((\lambda,\lambda')$ -Strong-Convexity)

The function $g(\mathbf{a}^*,\cdot)$ is λ -strongly convex, and $g(\cdot,\mathbf{b}^*)$ is λ' -strongly convex. That is, for any $\mathbf{b}_1,\mathbf{b}_2\in\mathcal{B}$ and $\mathbf{a}_1,\mathbf{a}_2\in\mathcal{A}$,

$$\begin{split} g(\textbf{a}^*,\textbf{b}_1) - g(\textbf{a}^*,\textbf{b}_2) - \left\langle \nabla_2 g(\textbf{a}^*,\textbf{b}_2), \textbf{b}_1 - \textbf{b}_2 \right\rangle & \geq & \frac{\lambda}{2} \cdot \|\textbf{b}_1 - \textbf{b}_2\|_2^2 \\ g(\textbf{a}_1,\textbf{b}^*) - g(\textbf{a}_2,\textbf{b}^*) - \left\langle \nabla_1 g(\textbf{a}_2,\textbf{b}^*), \textbf{a}_1 - \textbf{a}_2 \right\rangle & \geq & \frac{\lambda'}{2} \cdot \|\textbf{a}_1 - \textbf{a}_2\|_2^2 \end{split}$$



Theory: Population Version

Denote population minimization functions:

$$M_1(\mathbf{a}) = \arg\min_{\mathbf{b}} g(\mathbf{a}, \mathbf{b}); \quad M_2(\mathbf{b}) = \arg\min_{\mathbf{a}} g(\mathbf{a}, \mathbf{b}).$$

Condition $((\gamma, \gamma')$ -Lipschitz-Gradient)

The function $\nabla_2 g(\mathbf{a},\cdot)$ satisfies γ -Lipschitz gradient condition, and the function $\nabla_1 g(\cdot,\mathbf{b})$ satisfies γ' -Lipschitz gradient condition. That is, for any $\mathbf{a} \in \mathcal{A}$ and any $\mathbf{b} \in \mathcal{B}$,

$$\begin{split} &\left\|\nabla_2 g(\boldsymbol{a}^*, \textit{M}_1(\boldsymbol{a})) - \nabla_2 g(\boldsymbol{a}, \textit{M}_1(\boldsymbol{a}))\right\|_2 \leq \gamma \cdot \|\boldsymbol{a}^* - \boldsymbol{a}\|_2 \\ &\left\|\nabla_1 g(\textit{M}_2(\boldsymbol{b}), \boldsymbol{b}^*) - \nabla_1 g(\textit{M}_2(\boldsymbol{b}), \boldsymbol{b})\right\|_2 \leq \gamma^{'} \cdot \|\boldsymbol{b}^* - \boldsymbol{b}\|_2. \end{split}$$

Theory: Population Version

Theorem

Under (λ,λ') -Strong-Convexity and (γ,γ') -Lipschitz-Gradient conditions, we have

$$\left\| \textit{M}_{1}(a) - b^{*} \right\|_{2} \leq (\gamma/\lambda) \cdot \left\| a - a^{*} \right\|_{2} \; \textit{for any } a \in \mathcal{A},$$

$$\left\|\textit{M}_{2}(\textbf{b})-\textbf{a}^{*}\right\|_{2}\leq(\gamma^{'}/\lambda^{'})\cdot\left\|\textbf{b}-\textbf{b}^{*}\right\|_{2} \text{ for any } \textbf{b}\in\mathcal{B}.$$

Moreover, for any initialization $a^{\left(0\right)}$, the solutions from the population alternative updates converge linearly,

$$\left\|\mathbf{b}^{(t)} - \mathbf{b}^*\right\|_2 \leq (\frac{\gamma}{\lambda})^t (\frac{\gamma'}{\lambda'})^{t-1} \cdot \left\|\mathbf{a}^{(0)} - \mathbf{a}^*\right\|_2$$

$$\|\mathbf{a}^{(t)} - \mathbf{a}^*\|_2 \le (\frac{\gamma}{\lambda})^t (\frac{\gamma'}{\lambda'})^t \cdot \|\mathbf{a}^{(0)} - \mathbf{a}^*\|_2.$$

Theory: Sample Version

■ Denote sample minimization functions:

$$M_{1n}(\mathbf{a}) = \arg\min_{\mathbf{b}} g_n(\mathbf{a}, \mathbf{b}); \quad M_{2n}(\mathbf{b}) = \arg\min_{\mathbf{a}} g_n(\mathbf{a}, \mathbf{b}).$$

Condition (Statistical-Error(ϵ_s , δ , n))

Uniformly over all $\mathbf{a} \in \mathcal{A}$ with $\mathbf{b} \in \mathcal{B}$, we have that

$$\max \left\{ \left\| \mathit{M}_{1\mathit{n}}(\mathbf{a}) - \mathit{M}_{1}(\mathbf{a}) \right\|_{2}, \left\| \mathit{M}_{2\mathit{n}}(\mathbf{b}) - \mathit{M}_{2}(\mathbf{b}) \right\|_{2} \right\} \leq \epsilon_{\mathit{s}}$$

with probability at least $1 - \delta$.



Theory: Main Result

Denote the initialization error as $\epsilon_0 := \|\widehat{\mathbf{a}}_n^{(0)} - \mathbf{a}^*\|_2$.

Theorem

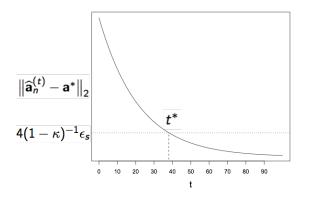
Under above assumptions and assume $\gamma < \lambda$ and $\gamma' < \lambda'$ s.t. $\kappa = \gamma \gamma' / (\lambda \lambda') < 1$. Assume $\widehat{\mathbf{a}}_n^{(0)} \in \mathcal{B}(\alpha; \mathbf{a}^*)$, and n is sufficiently large such that $\epsilon_s \leq \min\{(1-\gamma/\lambda)\alpha, (1-\gamma'/\lambda')\alpha\}$. Then

$$\|\widehat{\mathbf{b}}_{n}^{(t)} - \mathbf{b}^{*}\|_{2} \leq 2(1 - \kappa)^{-1} \epsilon_{s} + \kappa^{t-1} \epsilon_{0},$$

$$\|\widehat{\mathbf{a}}_{n}^{(t)} - \mathbf{a}^{*}\|_{2} \leq \underbrace{2(1 - \kappa)^{-1} \epsilon_{s}}_{Statistical\ Error} + \underbrace{\kappa^{t} \epsilon_{0}}_{Optimization\ Error}.$$

Theory: Main Result

$$\|\widehat{\mathbf{a}}_{n}^{(t)} - \mathbf{a}^*\|_{2} \le \underbrace{2(1-\kappa)^{-1}\epsilon_{s}}_{\text{Statistical Error}} + \underbrace{\kappa^{t}\epsilon_{0}}_{\text{Optimization Error}}$$



Application 1: Bigraphical model

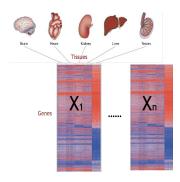


Figure: Matrix-variate data

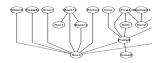


Figure : Gene network



Figure: Tissue network

Application 1: Bigraphical Model

A random matrix $\mathbf{X} \in \mathbb{R}^{p \times q}$ follows a matrix-variate normal if

$$\operatorname{vec}(\mathbf{X}) \sim N_{pq}(\mathbf{0}, \Psi \otimes \Sigma).$$

- Denote the precision matrices $\Lambda = \Psi^{-1}$ and $\Omega = \Sigma^{-1}$
- Zeros in Λ (or Ω) define pairwise conditional independence of corresponding entries given all other entries.
- Goal: Estimate sparse Λ and Ω .

Bigraphical Model

■ Given i.i.d. data $\mathbf{X}_1, \dots, \mathbf{X}_n$, the lasso penalized likelihood estimator minimizes

$$g_n(\Omega, \Lambda) = \frac{1}{n\rho q} \sum_{i=1}^n \operatorname{tr}(\boldsymbol{X}_i \Lambda \boldsymbol{X}_i^\top \Omega) - \frac{1}{\rho} \operatorname{logdet}(\Omega) - \frac{1}{q} \operatorname{logdet}(\Lambda) + \lambda_1 \|\Omega\|_1 + \lambda_2 \|\Lambda\|_1.$$

The population version likelihood function is

$$g(\Omega, \Lambda) = \frac{1}{\rho q} \mathbb{E} \big[\mathrm{tr} (\mathbf{X} \Lambda \mathbf{X}^\top \Omega) \big] - \frac{1}{\rho} \mathrm{logdet}(\Omega) - \frac{1}{q} \mathrm{logdet}(\Lambda).$$

■ The objective function $g(\Omega, \Lambda)$ is biconvex in (Ω, Λ) .

Bigraphical Model: Algorithm

Input: samples $\mathbf{X}_1, \dots, \mathbf{X}_n$, maximal number of iterations T, tuning parameters λ_1, λ_2 . **Initialize** $\Omega^{(0)}$.

For t = 1 to T: Alternatively update $\Omega^{(t)}$, $\Lambda^{(t)}$ as

lacksquare Given $\Omega^{(t-1)}$, compute $\mathbf{S}_1 = (np)^{-1} \sum_{i=1}^n \mathbf{X}_i^{ op} \Omega^{(t-1)} \mathbf{X}_i$ and solve the glasso problem

$$\Lambda^{(t)} = \arg\min_{\Lambda} \left\{ \frac{1}{q} \mathrm{tr}(\mathbf{S}_1 \Lambda) - \frac{1}{q} \mathrm{logdet}(\Lambda) + \lambda_{\Lambda} \|\Lambda\|_1 \right\}$$

 \blacksquare Given $\Lambda^{(t)}$, compute $\mathbf{S}_2=(nq)^{-1}\sum_{i=1}^n\mathbf{X}_i\Lambda^{(t)}\mathbf{X}_i^\top$ and solve the glasso problem

$$\boldsymbol{\Omega}^{(t)} = \arg\min_{\boldsymbol{\Omega}} \left\{ \frac{1}{\rho} \mathrm{tr}(\mathbf{S}_2 \boldsymbol{\Omega}) - \frac{1}{\rho} \mathrm{logdet}(\boldsymbol{\Omega}) + \lambda_{\boldsymbol{\Omega}} \|\boldsymbol{\Omega}\|_1 \right\}$$

End For

Output: $\widehat{\Omega} = \Omega^{(T)}$ and $\widehat{\Lambda} = \Lambda^{(T)}$.



- Step 1: Verify Strongly-Convexity of $g(\Omega^*, \cdot)$ and $g(\cdot, \Lambda^*)$, and Lipschitz-Gradient conditions of $\nabla_1 g(\cdot, \Lambda)$ and $\nabla_2 g(\Omega, \cdot)$.
- Define

$$\mathcal{B}(\alpha; \Omega^*) := \{ \Omega \in \mathbb{R}^{p \times p} : \|\Omega - \Omega^*\|_F \le \alpha \}$$

$$\mathcal{B}(\alpha; \Lambda^*) := \{ \Lambda \in \mathbb{R}^{q \times q} : \|\Lambda - \Lambda^*\|_F \le \alpha \}.$$

The alternative update algorithm via the population objective function $g(\Omega, \Lambda)$ is locally contractive.

Corollary

For the population objective function $g(\Omega, \Lambda)$, we have that $g(\Omega^*, \cdot)$ and $g(\cdot, \Lambda^*)$ are strongly convex with parameters, respectively,

$$\lambda = p^{-1}[\|\Omega^*\|_2 + 3\alpha]^{-2} \text{ and } \lambda' = q^{-1}[\|\Lambda^*\|_2 + 3\alpha]^{-2}.$$

Both $\nabla_1 g(\cdot,\Lambda)$ and $\nabla_2 g(\Omega,\cdot)$ satisfy the Lipschitz-Gradient conditions with

$$\gamma = \gamma' = (pq)^{-1} \|\Sigma^* \otimes \Psi^*\|_F.$$

If $\|\Sigma^* \otimes \Psi^*\|_F$ is bounded and if there exist constants $C_1, C_2 > 0$ such that $C_1 \leq \|\Omega^*\|_2, \|\Lambda^*\|_2 \leq C_2$, then

$$\gamma < \lambda, \gamma^{'} < \lambda^{'}$$
.



- Step 2: Compute the statistical error.
- Let $S_1 := \{(i,j) : \Omega_{ii}^* \neq 0\}$ and $S_2 := \{(i,j) : \Lambda_{ii}^* \neq 0\}$.
- Denote $s_1 = |S_1| p$ and $s_2 = |S_2| q$.
- Remind that

$$M_{1n}(\Omega) := \arg\min_{\Lambda} g_n(\Omega, \Lambda), \ M_{2n}(\Lambda) = \arg\min_{\Omega} g_n(\Omega, \Lambda),$$

 $M_1(\Omega) := \arg\min_{\Lambda} g(\Omega, \Lambda), \ M_2(\Lambda) = \arg\min_{\Omega} g(\Omega, \Lambda).$

Condition (Bounded Eigenvalues)

There are positive constants C_1 and C_2 such that

$$0 < C_1 \le \lambda_{\mathsf{min}}(\Sigma^*) \le \lambda_{\mathsf{max}}(\Sigma^*) \le 1/C_1 < \infty$$
$$0 < C_2 \le \lambda_{\mathsf{min}}(\Psi^*) \le \lambda_{\mathsf{max}}(\Psi^*) \le 1/C_2 < \infty.$$

Condition (Tuning)

The tuning parameters satisfy

$$\lambda_\Omega = O\left(\sqrt{\frac{\log p}{np^2q}}\right), \lambda_\Lambda = O\left(\sqrt{\frac{\log q}{npq^2}}\right).$$



Corollary

Under above two conditions, the statistical errors are

$$\sup_{\Omega \in \mathcal{B}(\alpha; \Omega^*)} \|M_{1n}(\Omega) - M_1(\Omega)\|_F = O_p\left(\sqrt{\frac{(q+s_2)\log q}{np}}\right),$$

$$\sup_{\Lambda \in \mathcal{B}(\alpha; \Lambda^*)} \|M_{2n}(\Lambda) - M_2(\Lambda)\|_F = O_p\left(\sqrt{\frac{(p+s_1)\log p}{nq}}\right).$$

- Step 1: Exploit the independence structure in $(\Omega^*)^{\frac{1}{2}}\mathbf{X}(\Lambda^*)^{\frac{1}{2}}$.
- Step 2: Use Talagrand inequality for the convergence rate of

$$(np)^{-1}\sum_{i=1}^{n}\mathbf{X}_{i}^{\top}\Omega\mathbf{X}_{i}-p^{-1}\mathbb{E}\big[\mathbf{X}^{\top}\Omega\mathbf{X}\big].$$



Bigraphical Model: Main Result

Combine above two Corollaries, we have

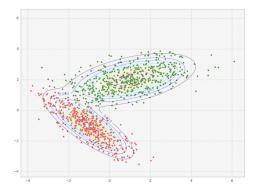
$$\begin{split} & \|\widehat{\Lambda}^{(t)} - \Lambda^*\|_F \leq C \sqrt{\frac{(p+s_1)\log p}{nq}} + \kappa^{t-1} \varepsilon_0, \\ & \|\widehat{\Omega}^{(t)} - \Omega^*\|_F \leq C \sqrt{\frac{(q+s_2)\log q}{np}} + \kappa^t \varepsilon_0. \end{split}$$

- When n = 1, we can still consistently estimate Λ^* or Ω^* .
- Leng and Tang (2012) showed there existed a local minimizer which can obtain above statistical error.
- We prove that our algorithm can find such minimizer.
- The convergence rates showed in Yin and Li (2012), Tsiligkaridis et al. (2013) are slower than ours and they require at least $n > (p+q)(\log p + \log q)$.



Application 2: Joint Clustering and Network Estimation

■ Gaussian mixture model (GMM) $\pi_k N(\mu_k, \Sigma_k)$, k = 1, ..., K.



Application 2: Background

- Samples $\mathbf{x}_i, \dots, \mathbf{x}_n$ follows a GMM with $\pi_k f_k(x; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$.
- If assume $\Sigma_k = \sigma_k \, \mathbb{1}_p$ (Pan and Shen, 2007, Sun et al., 2012), the clustering can be solved by minimizing

$$\sum_{i=1}^{n} \log \left(\sum_{k=1}^{K} \pi_k f_k(\mathbf{x}_i; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right) - P(\boldsymbol{\mu}).$$

 If assume clustering assignment is given, the networks are estimated jointly (Guo et al., 2011, Danaher et al., 2014) via

$$\max_{\substack{\Omega_1, \dots, \Omega_K \\ \text{s.t.}}} \quad \sum_{k=1}^K n_k [\log \det(\Omega_k) - \operatorname{tr}(S_k \Omega_k)] - P(\Omega)$$
s.t.
$$\Omega_1, \dots, \Omega_K \text{ are positive definite.}$$



Application 2: Joint Clustering and Network Estimation

■ Denote the set of parameters as $\Theta := \{(\mu_k, \Omega_k), k \in [K]\}$. Our optimization is formulated as

$$\max_{\pi_k, \mu_k, \Omega_k} \sum_{i=1}^n \log \left(\sum_{k=1}^K \pi_k f_k \left(\mathbf{x}_i; \boldsymbol{\mu}_k, \Omega_k \right) \right) - P(\Theta).$$

• We focus on the l_1 penalty on μ_k and fussed graphical lasso penalty (Danaher et al., 2014) on $\Omega_k = (\omega_{kij})$,

$$P(\Theta) = \lambda_1 \sum_{k=1}^{K} \sum_{j=1}^{p} |\mu_{kj}| + \lambda_2 \sum_{k=1}^{K} \sum_{i \neq j} |\omega_{kij}| + \lambda_3 \sum_{k < k'} \sum_{i,j} |\omega_{kij} - \omega_{k'ij}|.$$

Application 2: EM Algorithm

- Denote the K clusters as A_1, \dots, A_K , denote cluster assignment matrix L with entry $L_{ik} = \mathbf{1}(X_i \in A_k)$.
- The regularized complete log-likelihood function is

$$\log L_c(\Theta) := \sum_{i=1}^n \sum_{k=1}^K L_{ik} [\log \pi_k + \log f_k(x_i; \Theta_k)] - P(\Theta).$$

E-step: compute the conditional expectation

$$Q(\Theta|\widehat{\Theta}^{(t)}) := \sum_{i=1}^{n} \sum_{k=1}^{K} \widehat{L}_{ik}^{(t)} [\log \pi_k + \log f_k(x_i; \Theta_k)] - P(\Theta).$$

■ M-step: maximize $Q(\Theta|\widehat{\Theta}^{(t)})$ w.r.t. π_k , μ_k , Ω_k .



Application 2: EM Algorithm

M-step is a tri-convex optimization.

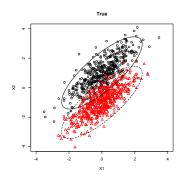
- Update π_k : $\widehat{\pi}_k^{(t+1)} = n^{-1} \sum_{i=1}^n \widehat{L}_{ik}^{(t)}$.
- Update μ_k : solve sparse mean via KKT condition.
- Update Ω_k : solve sparse networks via existing joint graphical lasso algorithms,

$$\max_{\Omega_1,...,\Omega_K} \sum_{k=1}^K n_k [\log \det(\Omega_k) - \operatorname{trace}(\widetilde{S}_k \Omega_k)] - P(\Omega).$$

Application 2: Illustration

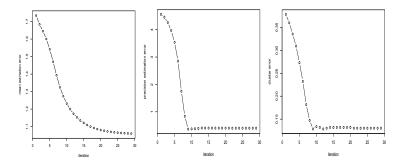
■ n = 1000 with 500 from $N(\mu_1, \Sigma)$ and 500 from $N(\mu_2, \Sigma)$,

$$\mu_1 = (0,1)^T, \mu_2 = (0,-1)^T, \Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}.$$



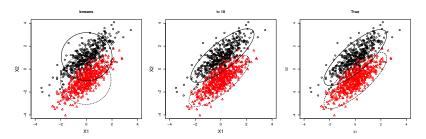
Application 2: Illustration

Figure : Mean vector estimation errors, precision matrix estimation errors, and cluster errors versus # of iterations.



Application 2: Illustration

Figure : Kmeans, Iteration t = 10 of our algorithm, and the truth.

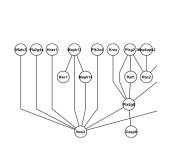


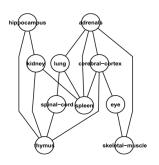
Summary

- A general convergence study of bi-convex problems.
- It reveals statistical and computational tradeoffs.
- Our theory is widely applicable to many models:
 - bigraphical model,
 - joint clustering and network estimation,
 - non-negative matrix factorization,
 - sparse tensor decomposition...

Future Work: Statistical Inference

- From parameter estimation to statistical inference.
- In the bigraphical model, test $H_0: \omega_{ij} = 0$ v.s. $H_1: \omega_{ij} \neq 0$
- Tools: Desparsify Lasso (van de Geer et al., 2014), De-correlated Score Test (Ning and Liu, 2014).







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