# A Fast and Scalable Joint Estimator for Learning Multiple Related Sparse Gaussian Graphical Models

Beilun Wang, Ji Gao, Yanjun Qi

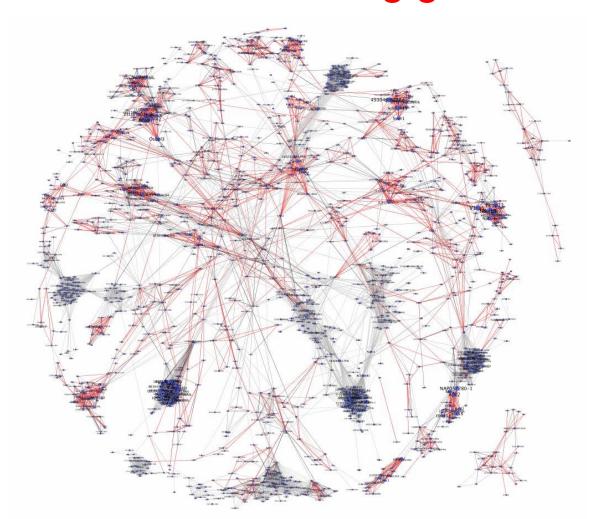
Proceedings of the 20th International Conference on Artificial Intelligence and Statistics (AISTAT17), PMLR 54:1168-1177, 2017.

```
R package: fasjem

http://jointggm.org
install.packages("fasjem")
library(fasjem)
demo(fasjem)
```

# Motivation: Entity Graph

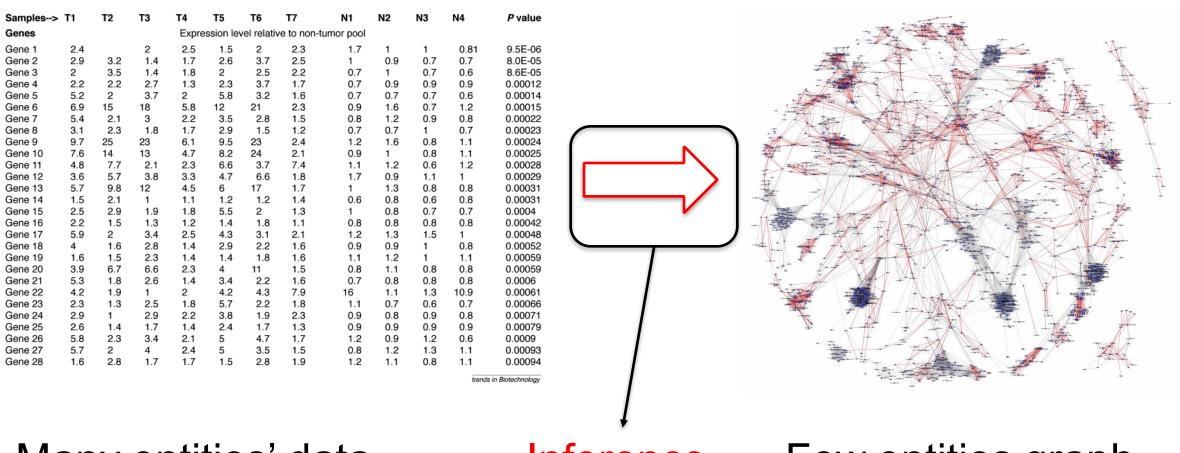
#### Interaction among genes





**Social Network** 

#### Motivation: Data to Graph

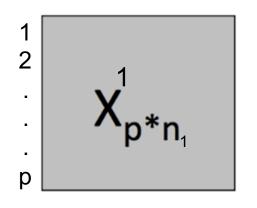


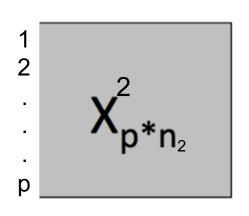
Many entities' data

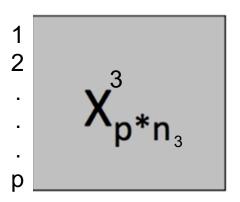
Inference Important Few entities graph

# Motivation: Data Heterogeneity across context

# Samples of the same set of genes(human genes) Vary across Normal vs Leukemia vs Stem







**Normal** 

Leukemia

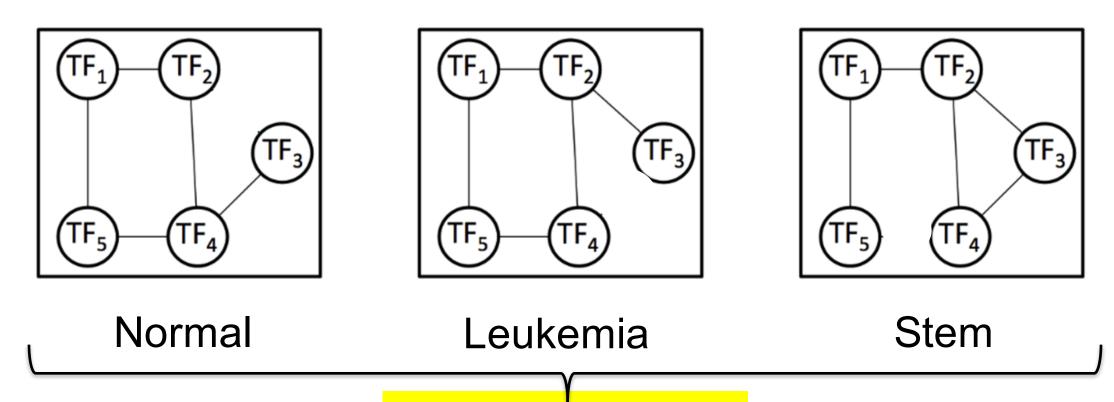
Stem

#### Notation

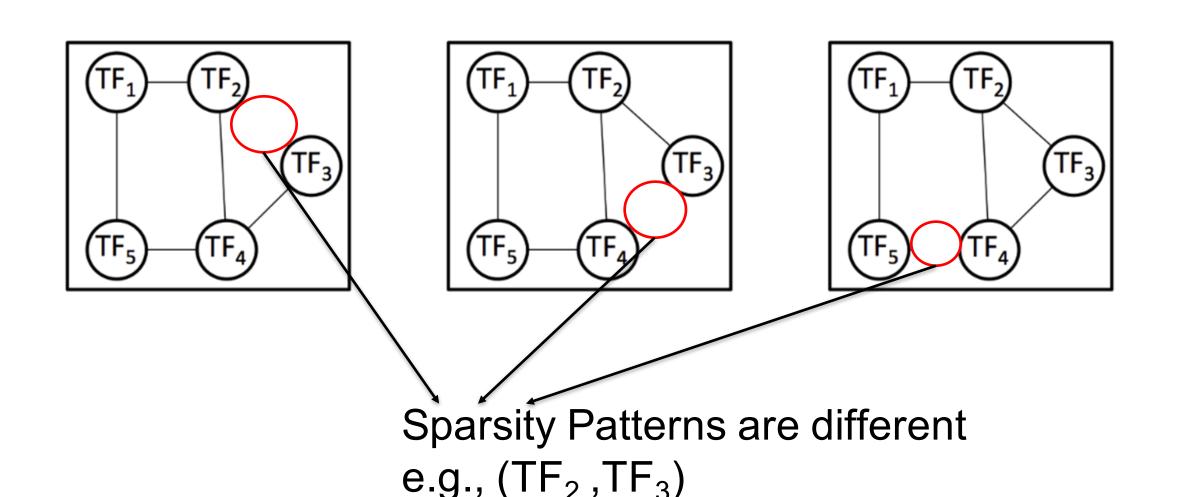
- p represents the number of nodes or features
- K represents the number of tasks or contexts

# Motivation: Entity Graphs vary across contexts

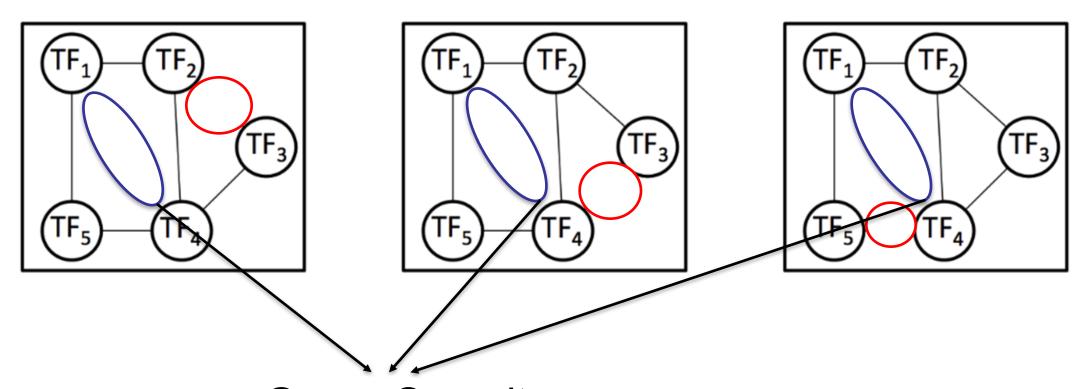
#### Different but related entity graphs



#### Difference among related graphs: Sparsity

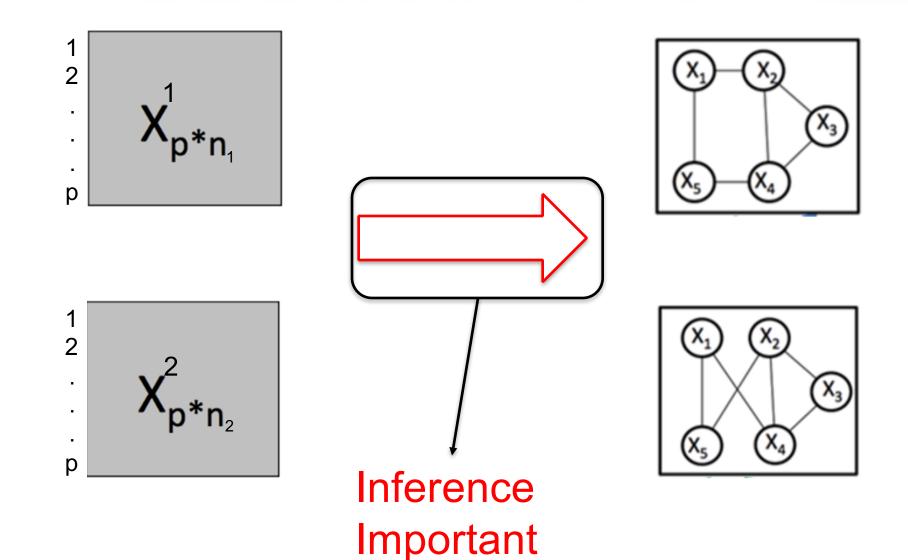


# Similarity among related graphs: Group Sparsity

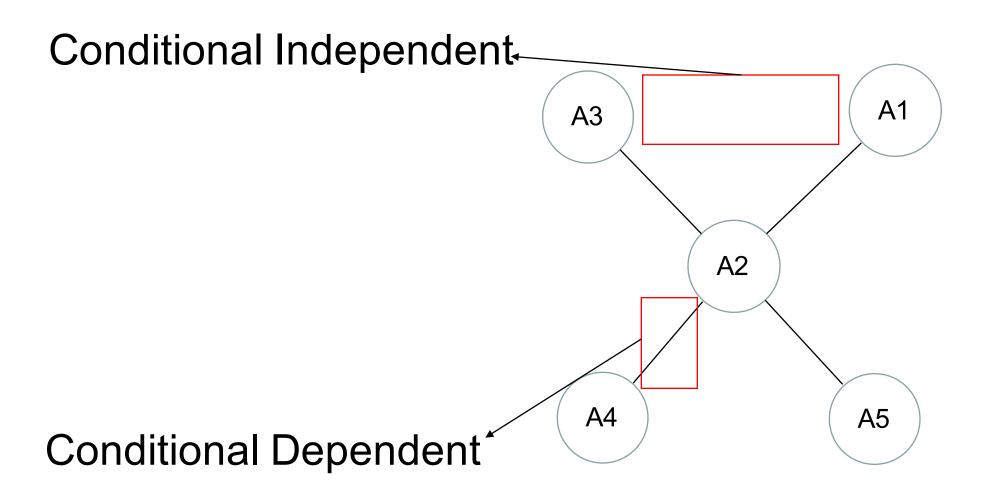


Group Sparsity means e.g., (TF<sub>1</sub>, TF<sub>4</sub>) no edge pattern across three

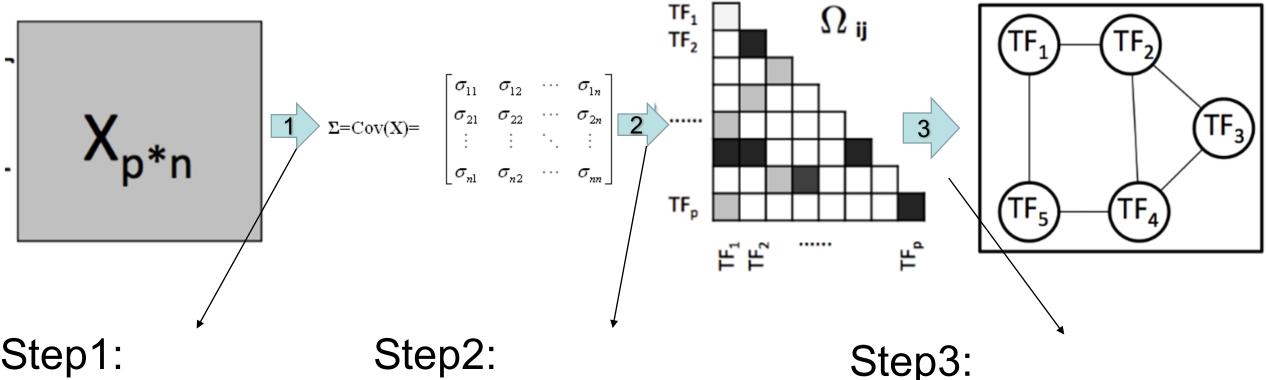
#### Motivation: Data to Graphs across context



# Motivation: Entity Graph — Conditional Independence Graph



#### Background: sparse Gaussian Graphical Model(sGGM) to derive Conditional Independence Graph from data



Step1:

Calculate the

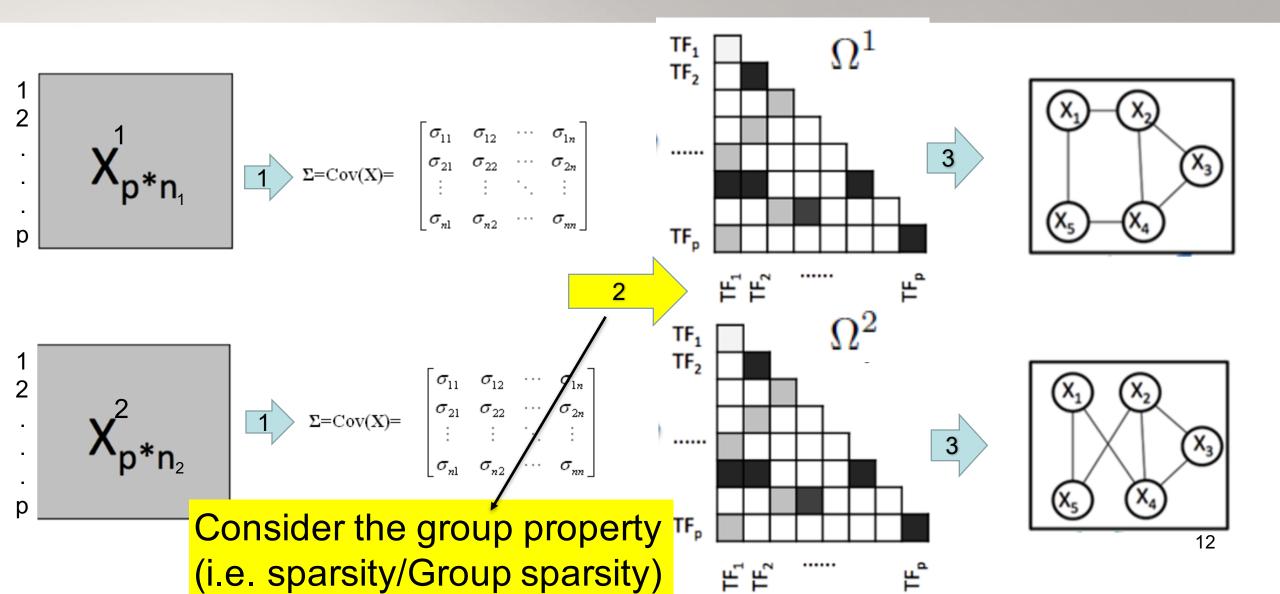
 $X \rightarrow \Sigma$ 

Step2:

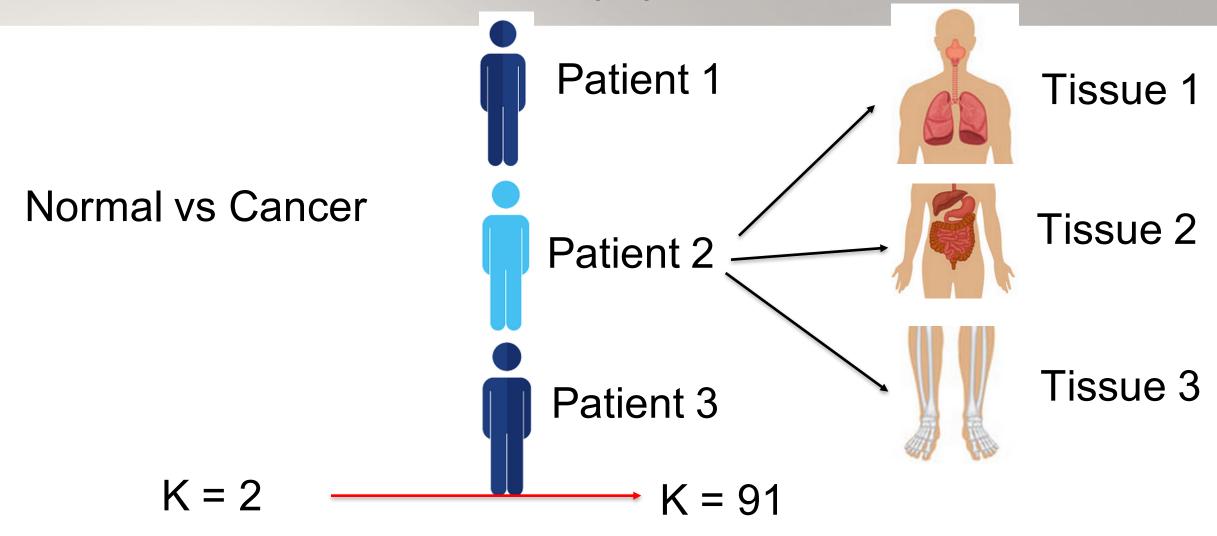
Estimate Sparse Inverse Transfer sparse matrix Covariance matrix of Covariance matrix

to Conditional Independence graph

#### Background Model: Multi-task sGGM



# Motivation: More tasks(K) to be considered



ENCODE Project Consortium et al. An integrated encyclopedia of dna elements in the human genome. *Nature*, 489(7414):57–74, 2012.

# Motivation: More Num of features(p) to consider

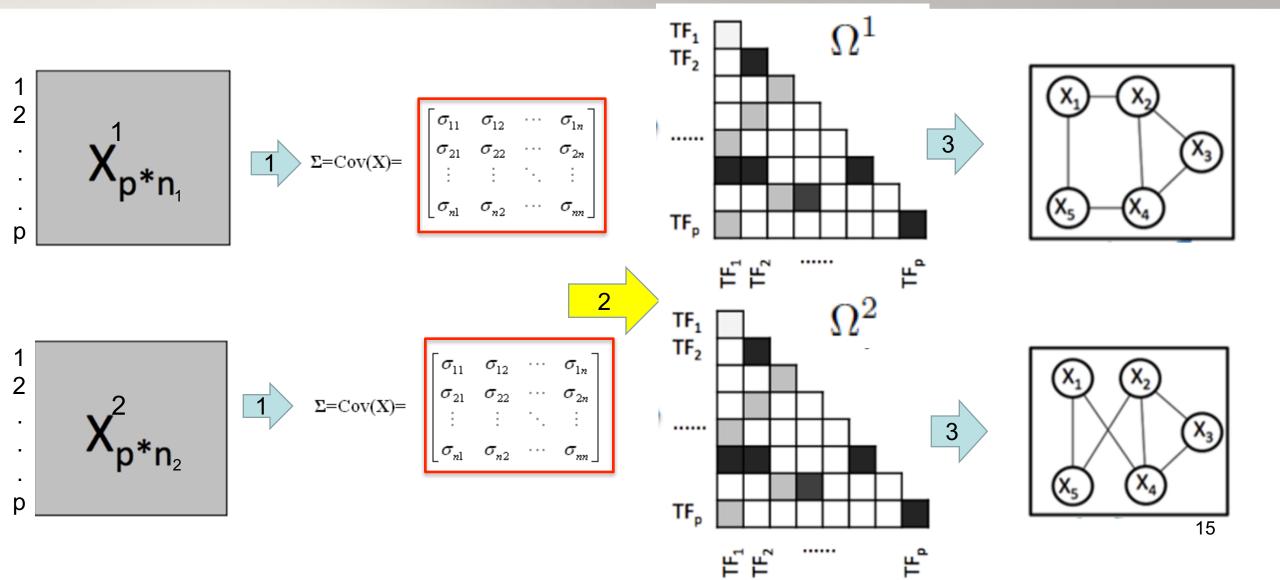
e.g. Yeast gene: 6K

Human gene: 30K



ENCODE Project Consortium et al. An integrated encyclopedia of dna elements in the human genome. *Nature*, 489(7414):57–74, 2012.

#### Limitation of Previous Methods: Storage



#### Limitation of Previous Methods: Storage

#### e.g., calculate the gradient

$$\mathbf{\Sigma} = \mathbf{Cov}(\mathbf{X}) = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn} \end{bmatrix}$$

$$\Sigma = \mathrm{Cov}(\mathbf{X}) = egin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \ dots & dots & \ddots & dots \ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn} \end{bmatrix}$$

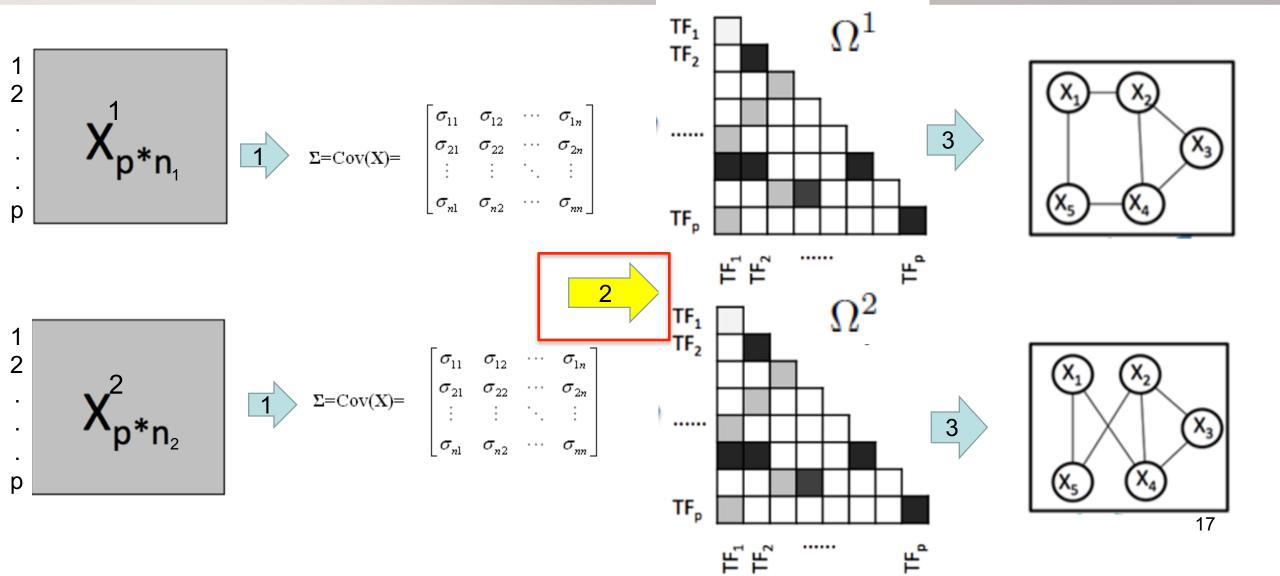
$$\Sigma = \text{Cov}(\mathbf{X}) = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn} \end{bmatrix}$$

$$K = 91, p = 30K$$

$$O(Kp^2)$$
 in memory

Double type: 65 TB

#### Limitation of Previous Methods: Speed



#### Limitation of Previous Methods: Speed

Suppose they have same iteration number T

**Traditional Optimization Method** 

$$K = 91, p = 30K$$

---- Block Coordinate Descent:

$$O(K^3p^4)$$
/ Itera

more than 2 billion years

Improved Optimization:

---- Still needs SVD for each covariance matrix

SVD for the matrices needs

$$O(Kp^3)$$
  $\longrightarrow$  3.5 days / Itera

#### Roadmap

- 1. Goal & Background
- 2. Proposed
- 3. Evaluation
- 4. Conclusion

#### Goal

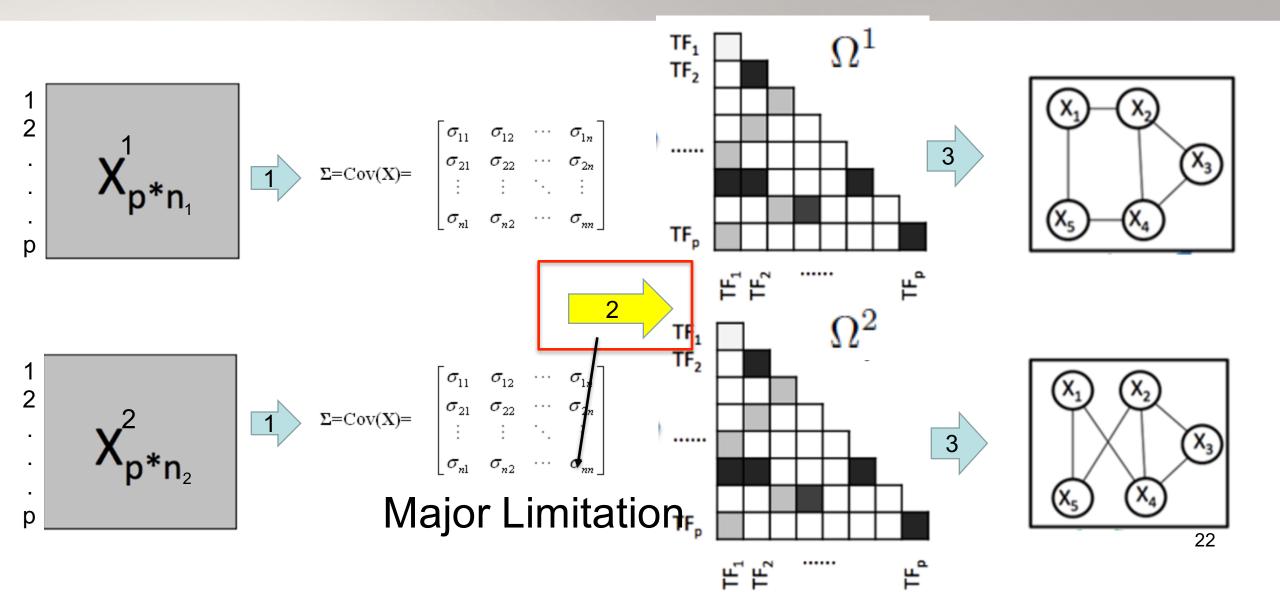
1. Design a fast and scalable joint estimator for multi-task sparse Gaussian Graphical Model

2. Prove the theoretical Bound for our estimator

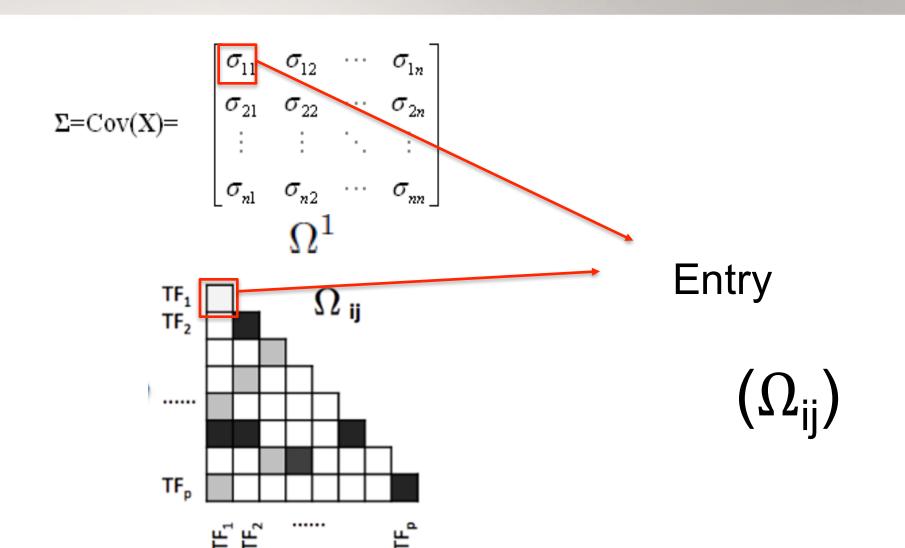
#### Roadmap

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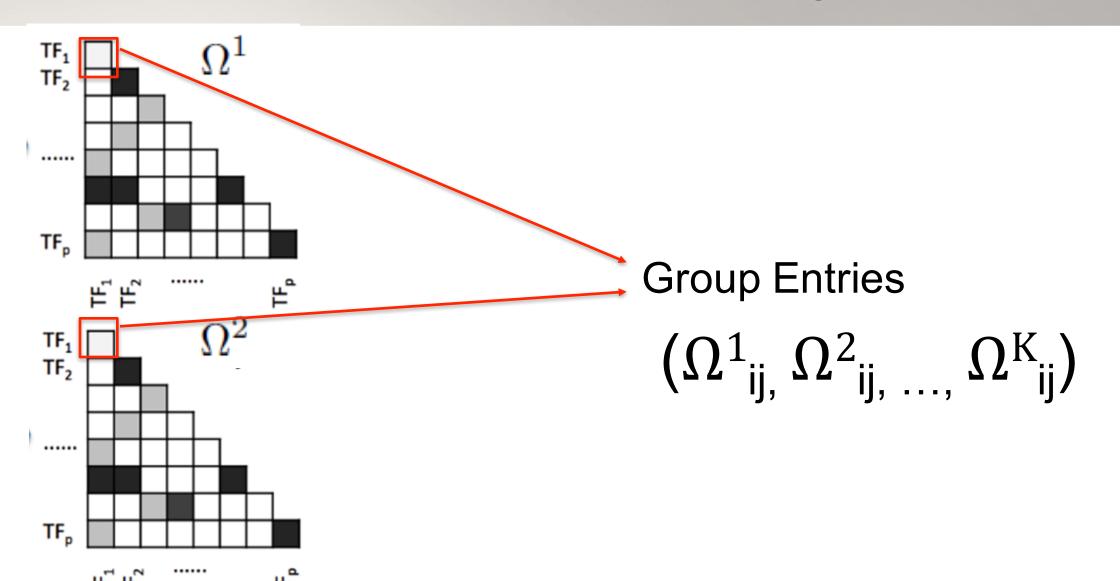
#### Major Limitation of Previous: Optimization



# Notation: Entry



#### Notation: Group Entries among all tasks



#### Our Model

✓ Traditional Models:

Penalized log-likelihood model ——— Better optimization method

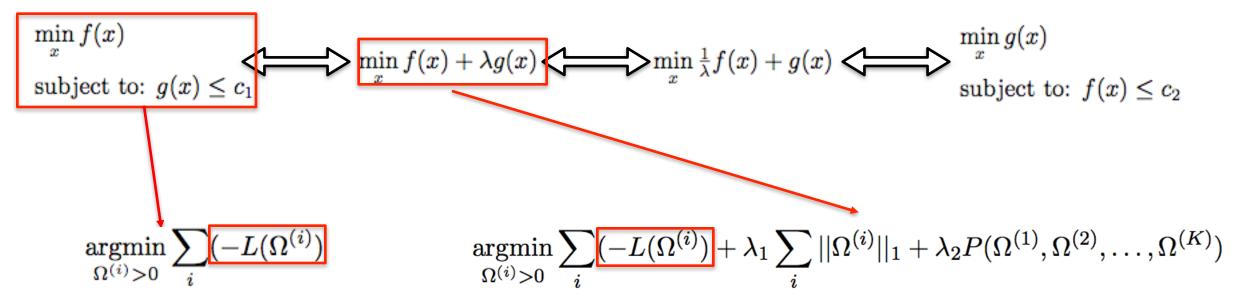
Some expensive computation is because of model itself!

✓ Proposed Model:

New model

Entry-wise(group entry-wise) optimization method

# Equivalent Forms of Constrained Optimization



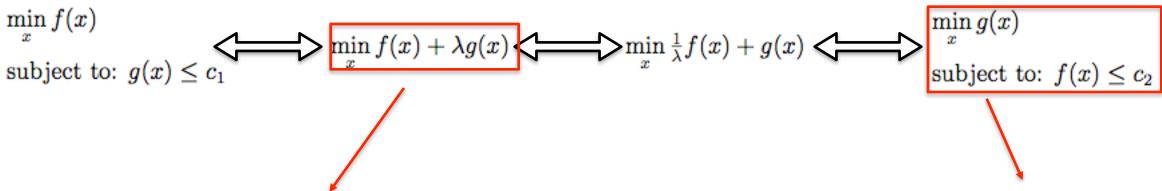
Subject to: 1. sparse

2. group sparse

**Traditional Models** 

Initial problem

# Equivalent Forms of Constrained Optimization



 $\underset{\Omega^{(i)}>0}{\operatorname{argmin}} \sum_{i} (-L(\Omega^{(i)}) + \lambda_1 \sum_{i} ||\Omega^{(i)}||_1 + \lambda_2 P(\Omega^{(1)}, \Omega^{(2)}, \dots, \Omega^{(K)})$ 

**Traditional Models** 

 $\underset{\Omega_{tot}}{\operatorname{argmin}} |\Omega_{tot}|_{1} + \epsilon R'(\Omega_{tot})$   $s.t. |\Omega_{tot} - inv(T_{v}(\Sigma_{tot}))|_{\infty} \leq \lambda_{n}$   $\mathcal{R}'^{*}(\Omega_{tot} - inv(T_{v}(\Sigma_{tot}))) \leq \epsilon \lambda_{n}$ 

**Proposed Models** 

#### Our Model: FASJEM

Fast and Scalable Joint Estimator for Multiple related sparse Gaussian Graphical Model

$$\underset{\Omega_{tot}}{\operatorname{argmin}} |\Omega_{tot}|_{1} + \epsilon R'(\Omega_{tot})$$

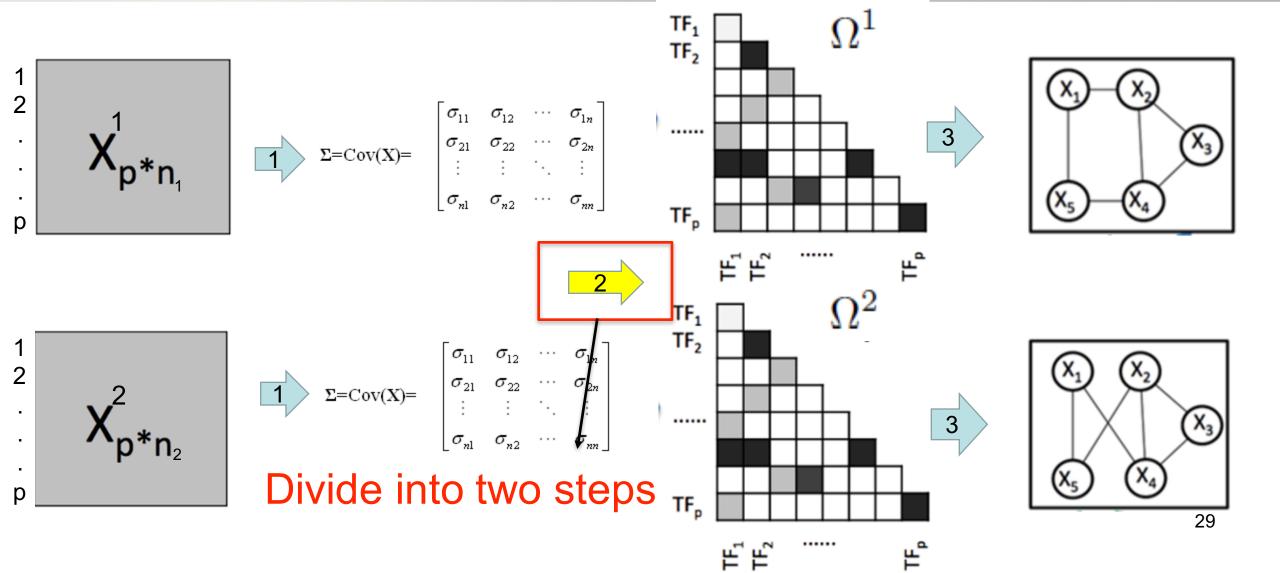
$$s.t. |\Omega_{tot} - inv(T_{v}(\Sigma_{tot}))|_{\infty} \leq \lambda_{n}$$

$$\mathcal{R}'^{*}(\Omega_{tot} - inv(T_{v}(\Sigma_{tot}))) \leq \epsilon \lambda_{n}$$

Here R' is another penalty norm and R'\* is the dual norm of R'

$$\Omega_{tot} = (\Omega^{(1)}, \Omega^{(2)}, \dots, \Omega^{(K)})$$
  $\Sigma_{tot} = (\Sigma^{(1)}, \Sigma^{(2)}, \dots, \Sigma^{(K)})$ 

#### Optimization: Structure



#### Optimization: Structure

• Step I: Pre-compute and pre-store(not in the memory) approximated backward mapping matrix  $\mathcal{B}^*(\Sigma_{tot})$ 

$$\Sigma_{tot}$$
  $\mathcal{B}^*(\Sigma_{tot})$ 

• Step II: Use proximity algorithm(entry-wise and group entry-wise) to solve the optimization problem.

$$\mathcal{B}^*(\Sigma_{tot}) \longrightarrow \Omega_{tot}$$

#### Optimization: Structure

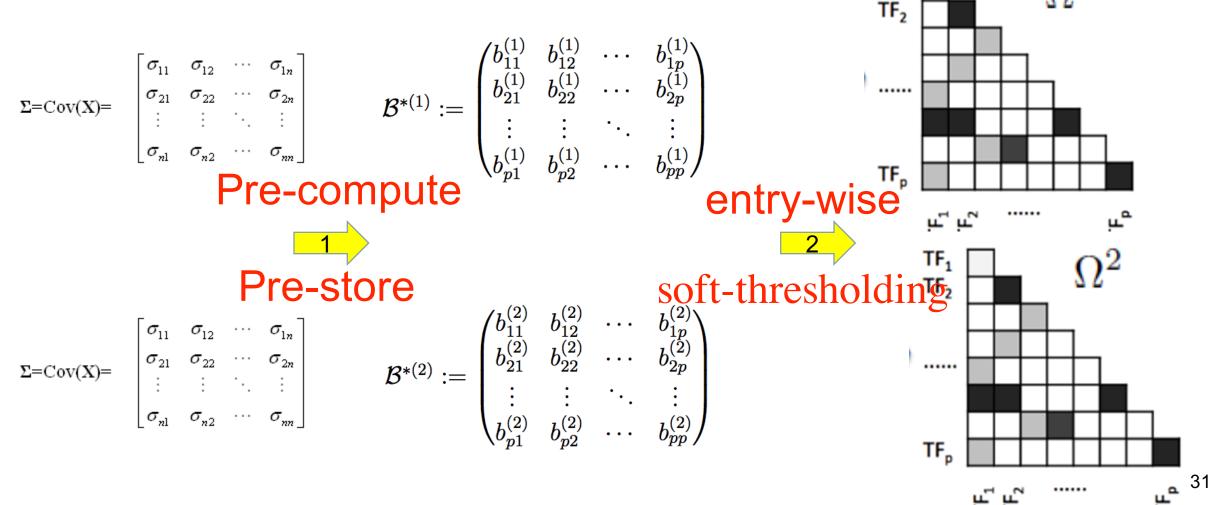
$$\Sigma = \text{Cov}(X) = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn} \end{bmatrix}$$

$$\mathcal{B}^{*(1)} := egin{pmatrix} b_{11}^{(1)} & b_{12}^{(1)} & \cdots & b_{1p}^{(1)} \ b_{21}^{(1)} & b_{22}^{(1)} & \cdots & b_{2p}^{(1)} \ dots & dots & \ddots & dots \ b_{p1}^{(1)} & b_{p2}^{(1)} & \cdots & b_{pp}^{(1)} \end{pmatrix}$$



$$\Sigma = \mathrm{Cov}(\mathrm{X}) = egin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \ \vdots & \vdots & \ddots & \vdots \ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn} \end{bmatrix}$$

$$\mathcal{B}^{*(2)} := egin{pmatrix} b_{11}^{(2)} & b_{12}^{(2)} & \cdots & b_{1p}^{(2)} \ b_{21}^{(2)} & b_{22}^{(2)} & \cdots & b_{2p}^{(2)} \ dots & dots & \ddots & dots \ b_{p1}^{(2)} & b_{p2}^{(2)} & \cdots & b_{pp}^{(2)} \end{pmatrix}$$



# Optimization: Step I

Precompute 
$$\mathcal{B}^*(\Sigma_{tot}) = inv(T_v(\Sigma_{tot}))$$

A matrix inversion + A soft-thresholding operator

Note: this only compute and pre-store(no need to store them in the memory) once. No need to use the whole matrix  $\Sigma_{tot}$  repeatedly.

Here 
$$inv(\Sigma_{tot}) := (\Sigma^{(1)^{-1}}, \Sigma^{(2)^{-1}}, \dots, \Sigma^{(K)^{-1}})$$

#### Optimization: Step2

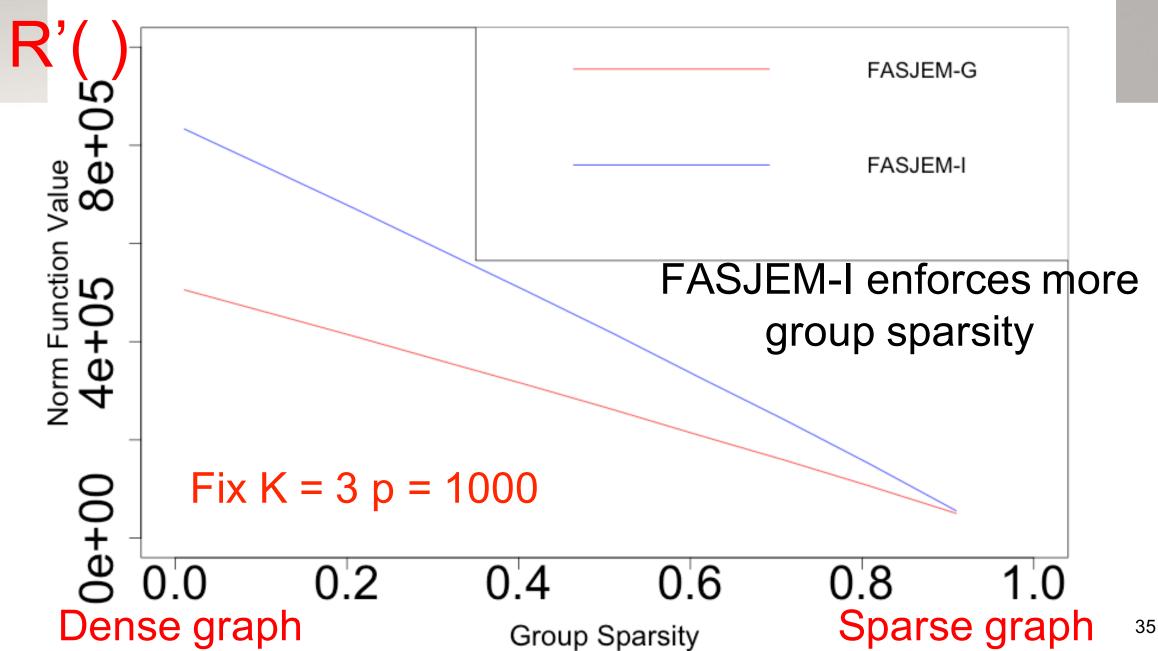
#### **Two Variations**

Case I -- FASJEM-G:

$$\mathcal{R}'(\cdot) = |\cdot|_{\mathcal{G},2}$$

Case II – FASJEM-I:

$$R'(\cdot) = |\cdot|_{\mathcal{G},\infty}$$



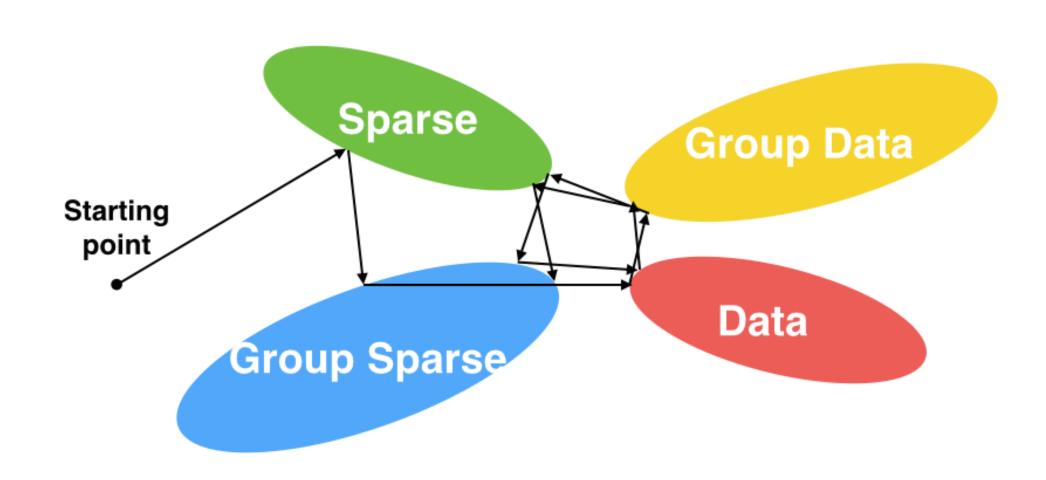
#### Optimization: Step II for FASJEM-G

We only need to compute the following four soft-thresholding operators for each entry(element) or group entries(element)

We choose FASJEM-G as an example.

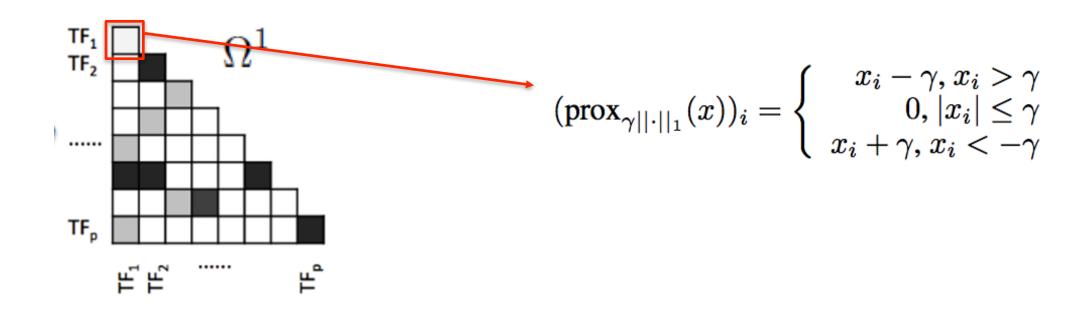
Other second norm is similar to this one.

#### Optimization Step2: Overall

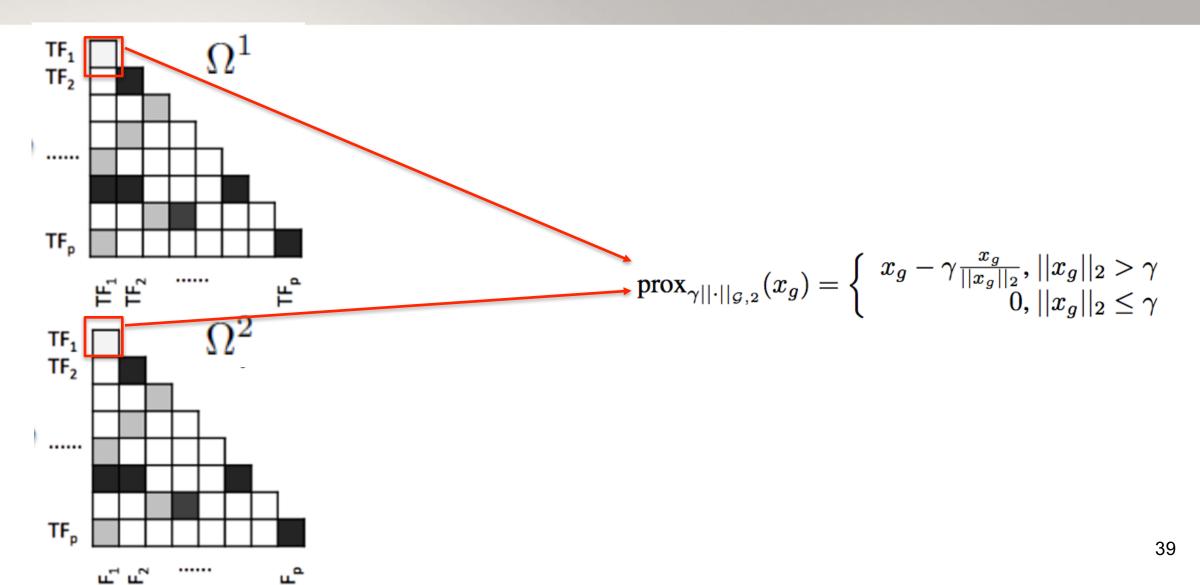


#### Optimization: Step II(1) - Sparse

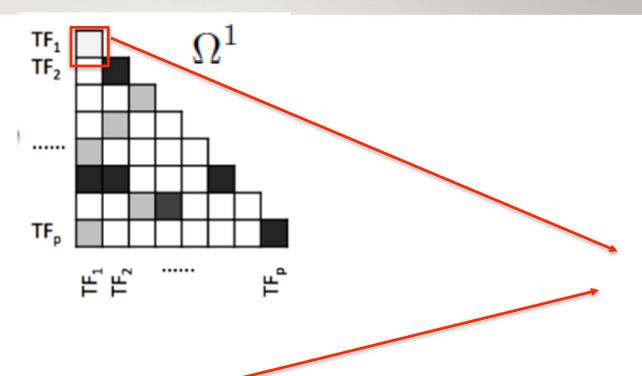
In each iteration,



#### Optimization: Step II(2) – Group sparse



#### Optimization: Step II (3) – Data

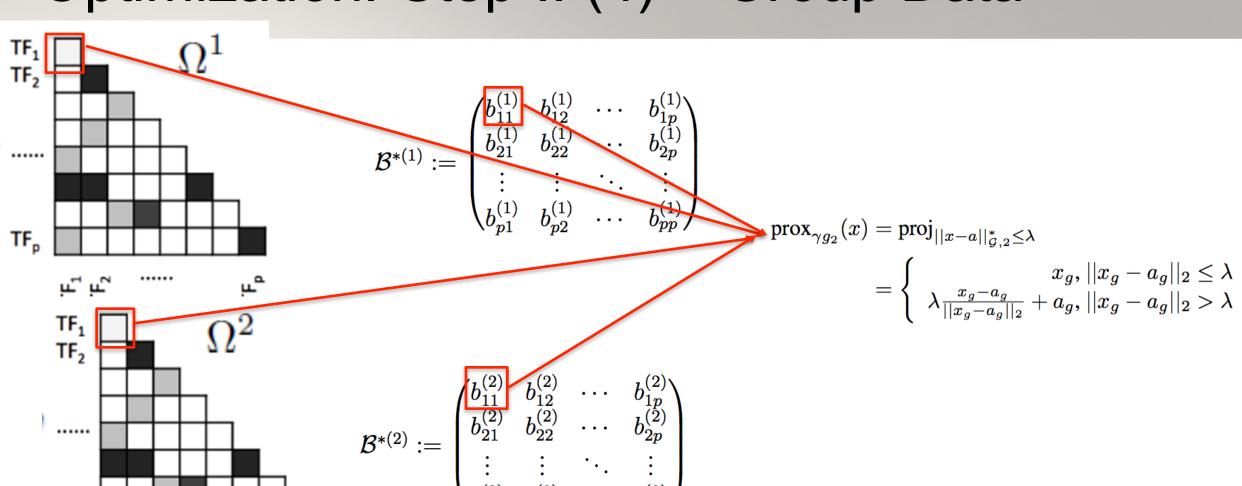


$$\operatorname{proj}_{||x-a||_{\infty} \leq \lambda} = \left\{egin{array}{l} x_i, |x_i-a_i| \leq \lambda \ a_i+\lambda, x_i > a_i+\lambda \ a_i-\lambda, x_i < a_i-\lambda \end{array}
ight.$$

$$\mathcal{B}^{*(1)} := egin{pmatrix} b_{11}^{(1)} & b_{12}^{(1)} & \cdots & b_{1p}^{(1)} \ b_{21}^{(1)} & b_{22}^{(1)} & \cdots & b_{2p}^{(1)} \ dots & dots & \ddots & dots \ b_{p1}^{(1)} & b_{p2}^{(1)} & \cdots & b_{pp}^{(1)} \end{pmatrix}$$

## Optimization: Step II (4) – Group Data

 $\mathsf{TF}_{\mathsf{p}}$ 



#### Advantage of Optimization: Space

Suppose they have same iteration number T

$$K = 91, p = 30K$$

Double type: 65 TB



Double type: 728B < 1KB

#### Advantage of Optimization: Time

Suppose they have same iteration number T

$$K = 91, p = 30K$$

Previous Multi-sGGM 
$$\longrightarrow$$
 (SVD) needs $O(Kp^3)$ / Itera

Totally entry-wise,  $O(Kp^2)$ / Itera also can be paralled

300000 times faster

3.5 days



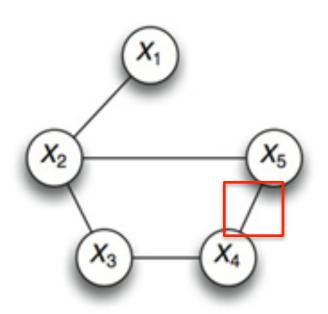
1 second

#### Roadmap

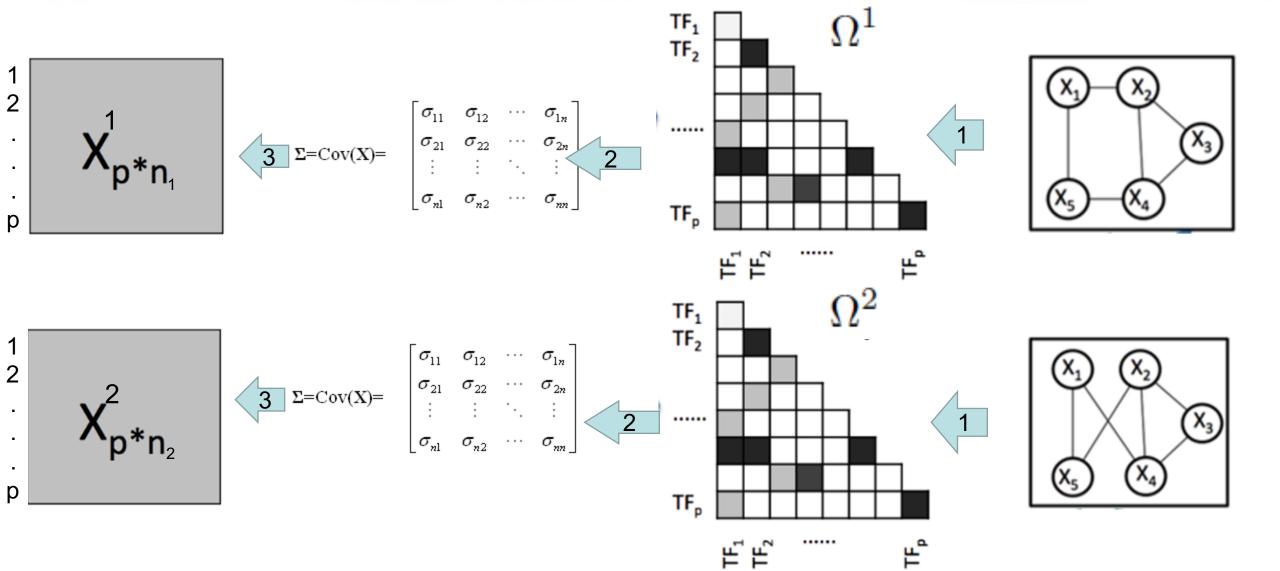
- 1. Goal & Background
- 2. Proposed
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#### My Work: Evaluation

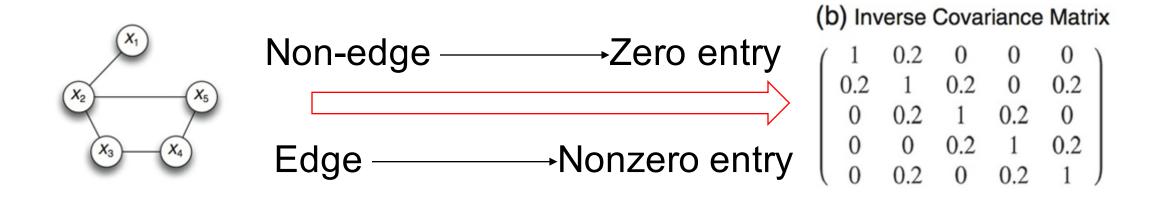
- 1. Simulation test
  - random graph models
- 2. Real world datasets
- 3. Theoretical Performance
  - e.g., Convergence rate



Generate edges randomly by Bernoulli distribution with probability q



#### Step1:



#### Step2:

$$\begin{bmatrix} 1 & 0.2 & 0 & 0 & 0 \\ 0.2 & 1 & 0.2 & 0 & 0.2 \\ 0 & 0.2 & 1 & 0.2 & 0 \\ 0 & 0 & 0.2 & 1 & 0.2 \\ 0 & 0.2 & 0 & 0.2 & 1 \end{bmatrix}$$
 
$$= \begin{bmatrix} 1.05 & -0.23 & 0.05 & -0.02 & 0.05 \\ -0.23 & 1.45 & -0.25 & 0.10 & -0.25 \\ 0.05 & -0.25 & 1.10 & -0.24 & 0.10 \\ -0.02 & 0.10 & -0.24 & 1.10 & -0.24 \\ 0.05 & -0.25 & 0.10 & -0.24 & 1.10 \end{bmatrix}$$
 Inverse

Step3:

Suppose  $X \sim N(\mu, \Sigma)$  and X is a p-dimensional vector

Use MCMC to simulate data set based on Covariance matrix

#### Evaluation: metric

1. ROC curve varying different tuning parameter, compare AUC(area under curve)

- 2. computation time
  - fix K varying p
  - fix p varying K
- 3. memory
  - how large p and K will cause the programme to terminate

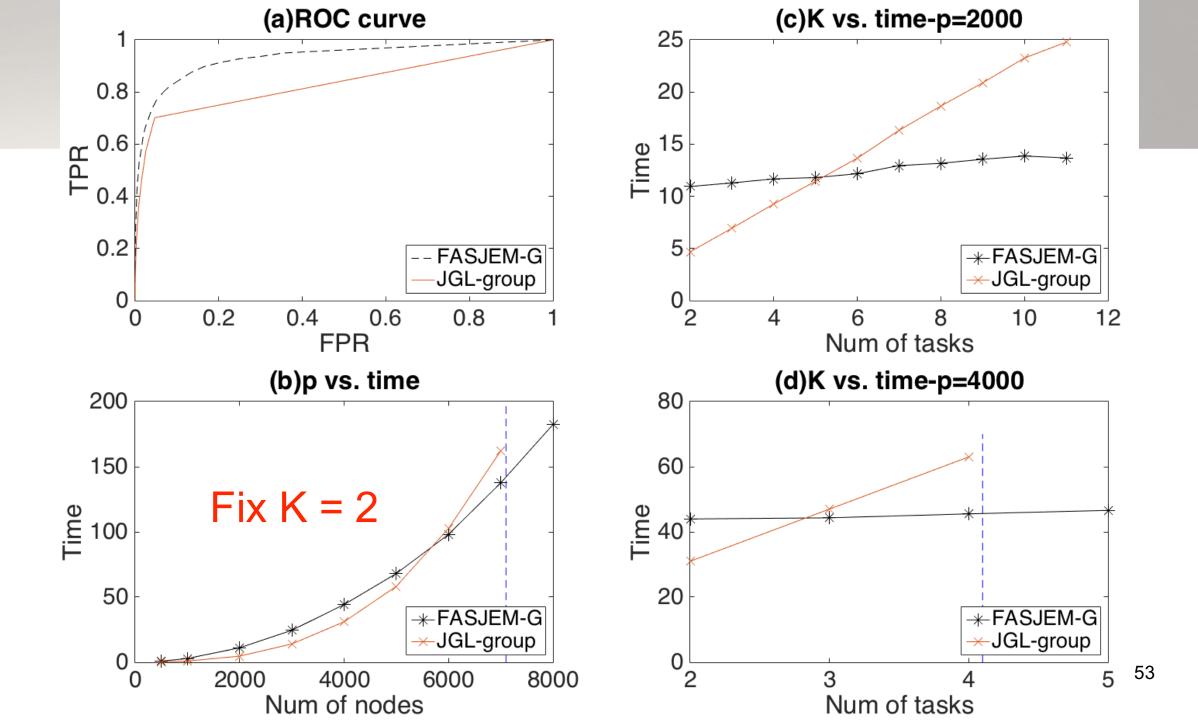
## Evaluation: Experimental Setting

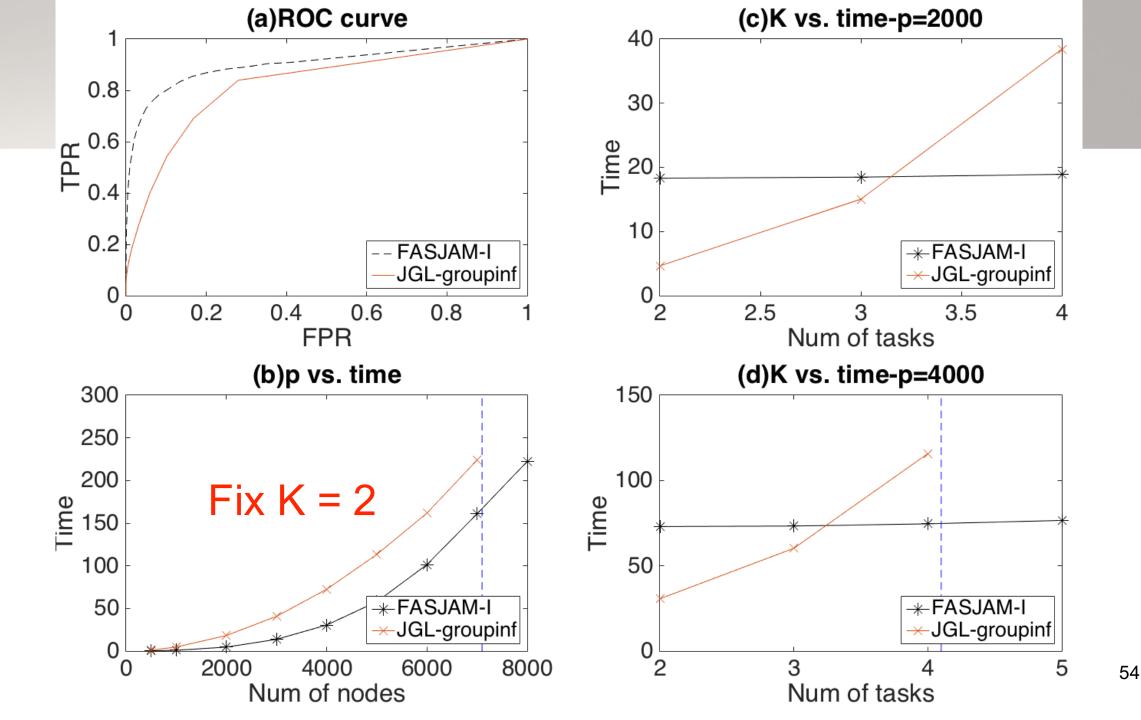
- simulation test datasets:
  - Model: random sparse graph model
  - Case I -- FASJEM-G:

$$\mathcal{R}'(\cdot) = |\cdot|_{\mathcal{G},2}$$

Case II – FASJEM-I:

$$R'(\cdot) = |\cdot|_{\mathcal{G},\infty}$$





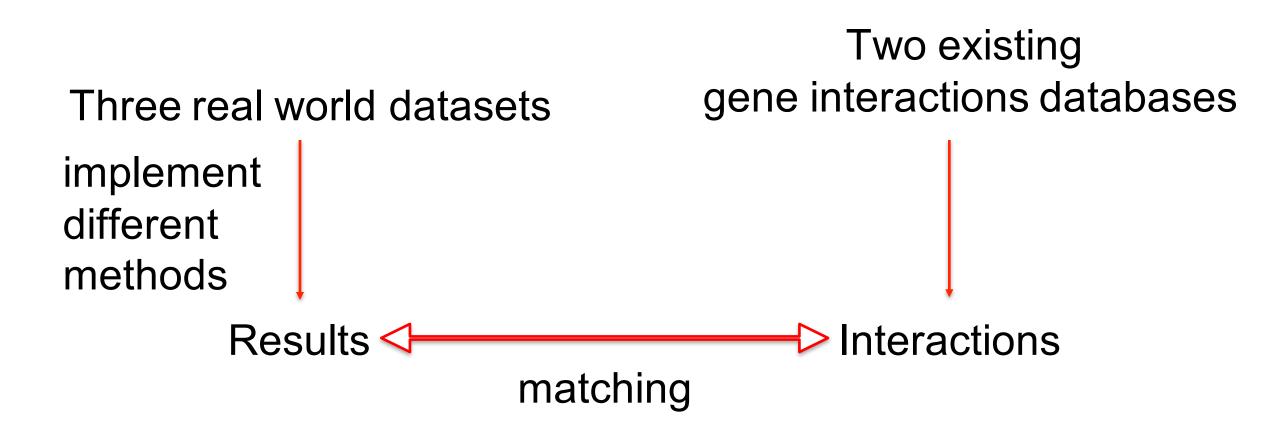
## Evaluation-Experiment Result I

Our models obtain the best accuracy result.

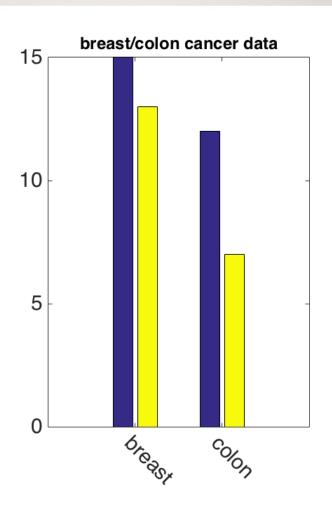
 Our models are faster than the baseline methods when p>6000&K=2 or p = 2000&K > 6

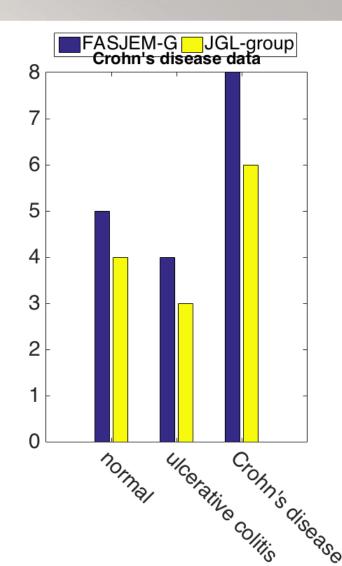
- Our models still work when p>8000&K=2 or p=4000&K>4
  - On 8GB memory desktop

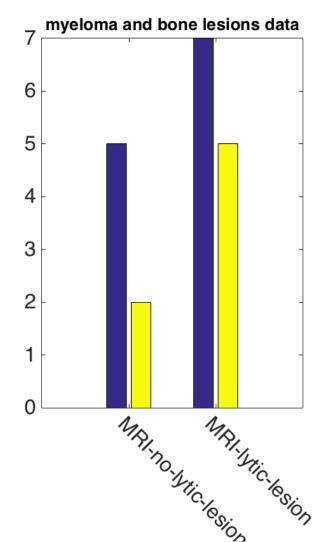
## Evaluation-Experiment Result II



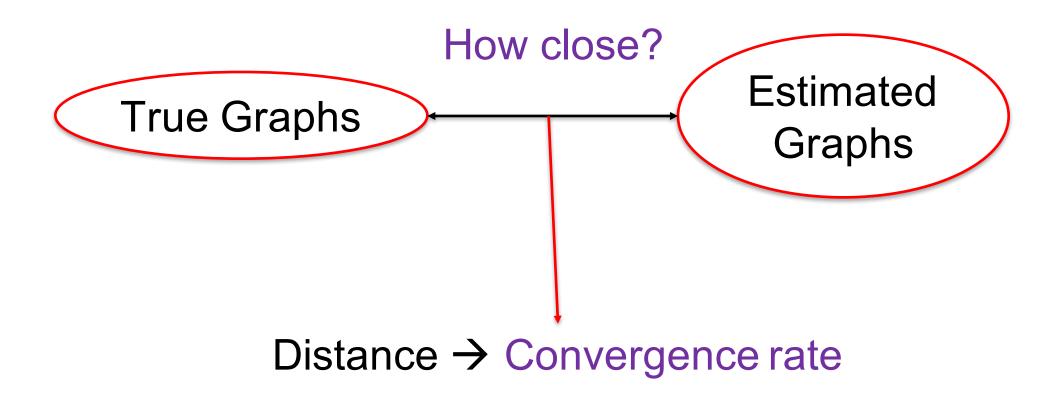
#### Evaluation-Experiment Result II







#### **Evaluation-Theoretical Analysis**



## Theoretical Analysis – Best convergence rate

General case > some experiments

The best convergence rate:

$$|\widehat{\mu} - \mu^*|_F \le 8 \max\{M_1 \sqrt{\frac{k_1 \log Kp}{n_{tot}}}, M_2 \sqrt{\frac{k_2 p \log Kp}{n_{tot}}}\}$$

Sahand Negahban, Bin Yu, Martin J Wainwright, and Pradeep K Ravikumar. A unified framework for high-dimensional analysis of m-estimators with decom- posable regularizers. In *Advances in Neural Information Processing Systems*, pages 1348–1356, 2009

## Theoretical Analysis – Best convergence rate

General cases' conclusion

The best convergence rate:

$$|\widehat{\mu} - \mu^*|_F \le 8 \max\{M_1 \sqrt{\frac{k_1 \log Kp}{n_{tot}}}, M_2 \sqrt{\frac{k_2 p \log Kp}{n_{tot}}}\}$$

We prove it!

# Theoretical Analysis – When compared to single task case

Single task:

$$|\widehat{\mu} - \mu^*|_F \le O(\sqrt{\frac{\log p}{n}})$$

Our case:

$$|\widehat{\mu} - \mu^*|_F \le 8 \max\{M_1 \sqrt{\frac{k_1 \log Kp}{n_{tot}}}, M_2 \sqrt{\frac{k_2 p \log Kp}{n_{tot}}}\}$$

#### Theoretical Analysis – Multi-task helps!

Suppose  $n_i = n_1$ 

$$\frac{\log Kp}{Kn_1} \le \frac{\log p}{n_1}$$

$$K = 91, p = 30K, n_1 = 1K$$

Our case 0.0001 << 0.01 Single case

Multi-task —> n increase —> closer distance

#### Conclusion

- We design a novel algorithm to solve the Multi-task sGGM
- We have the best simulation test result in
  - Accuracy
  - Time
  - Memory
- Our method achieve the best convergence rate

## Thank You!

http://jointggm.org

R package: fasjem

install.packages("fasjem")
library(fasjem)
demo(fasjem)

## Background: Multi-task sGGM to derive Conditional Independence Graph from data

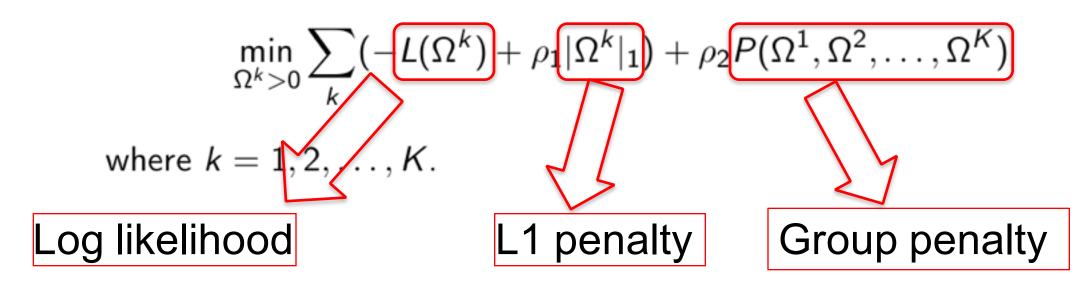
#### Step1:

Suppose  $X \sim N(\mu, \Sigma)$  and X is a p-dimensional vector

$$\widehat{\Sigma} = (X - \bar{X})^T (X - \bar{X})$$

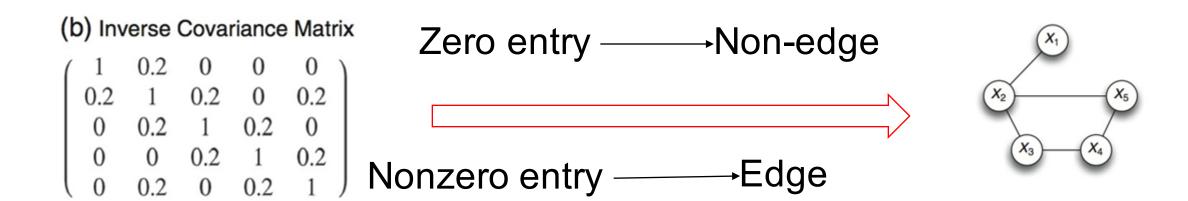
## Background: Multi-task sGGM to derive Conditional Independence Graph from data

Step2: We solve the following optimization problem:



## Background: Multi-task sGGM to derive Conditional Independence Graph from data

#### Step3:



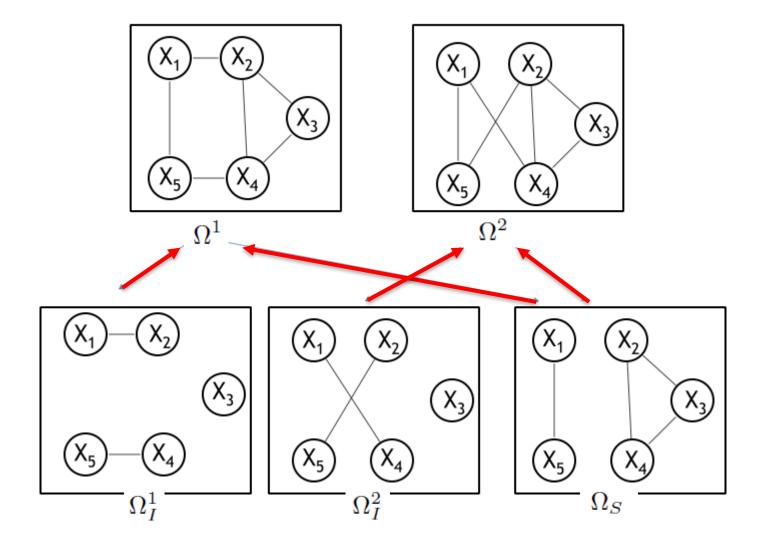
#### Background: Dual Norm

$$\mathcal{R}^*(v) := \sup_{u \in \mathbb{R}^p \setminus \{0\}} \frac{\langle u, v \rangle}{\mathcal{R}(u)} = \sup_{\mathcal{R}(u) \le 1} \langle u, v \rangle$$

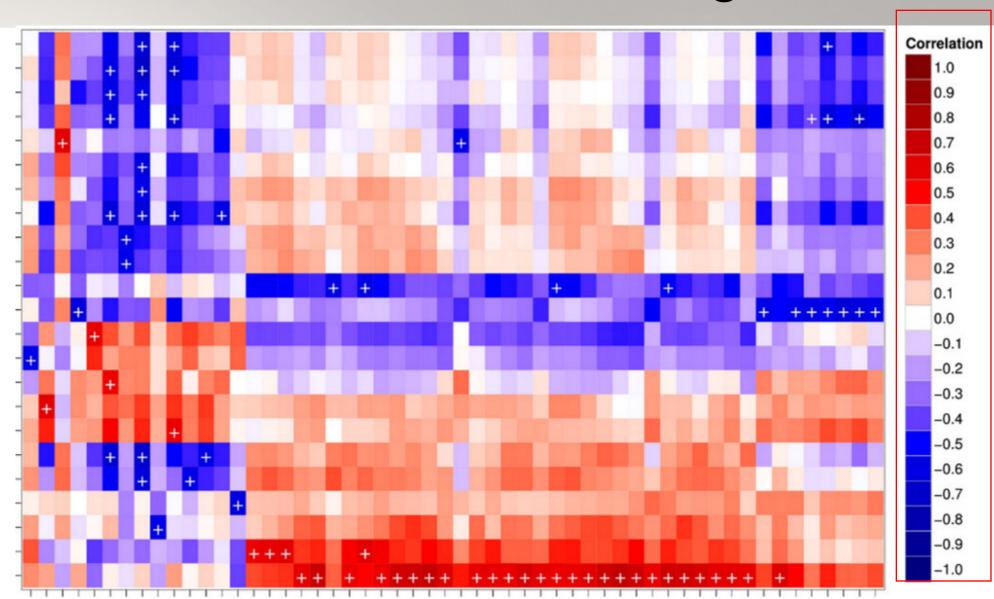
#### Experiment: Real world datasets

- (1) The breast/colon cancer data (with 2 cell type and 104 samples, each of which has 22283 features);
- (2) Chrohn's disease data (with 3 cell type and 127 samples, each of which has 22283 features)
- (3) The myeloma and bone lesions data set (with 2 cell type and 173 samples, each of which has 12625 features)
  - We select top 500 features based variable variance for all three datasets.

# Experiment: Synthesizing Data With Random Graph Model



Correlation Heatmap:



#### Example:

If X is a random variable follows N(0,1), let  $Y=X^2$ .

Then Cor(X,Y) = 0, but X and Y have dependent relationship.



A1: Children try swim

A1

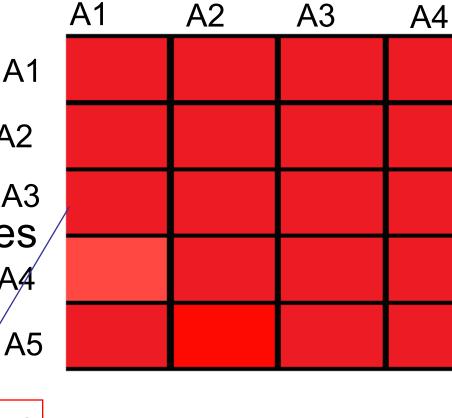
A2: Weather is hot A2

A3: High sale of ice cream A3

A4: Wear less amount of clothes

A5: High Electricity

Consumption



Correlation

0.7 0.6

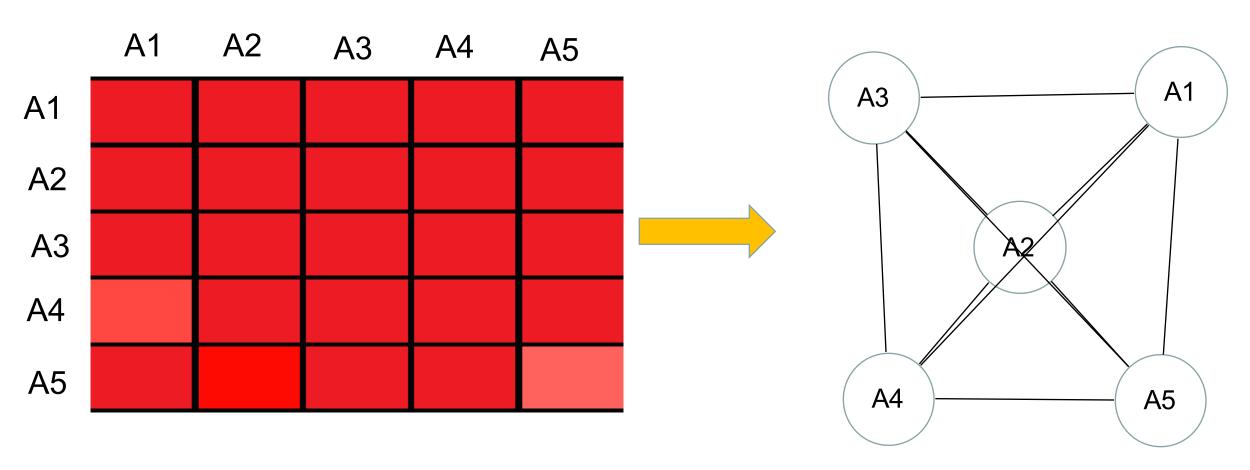
0.5

0.0

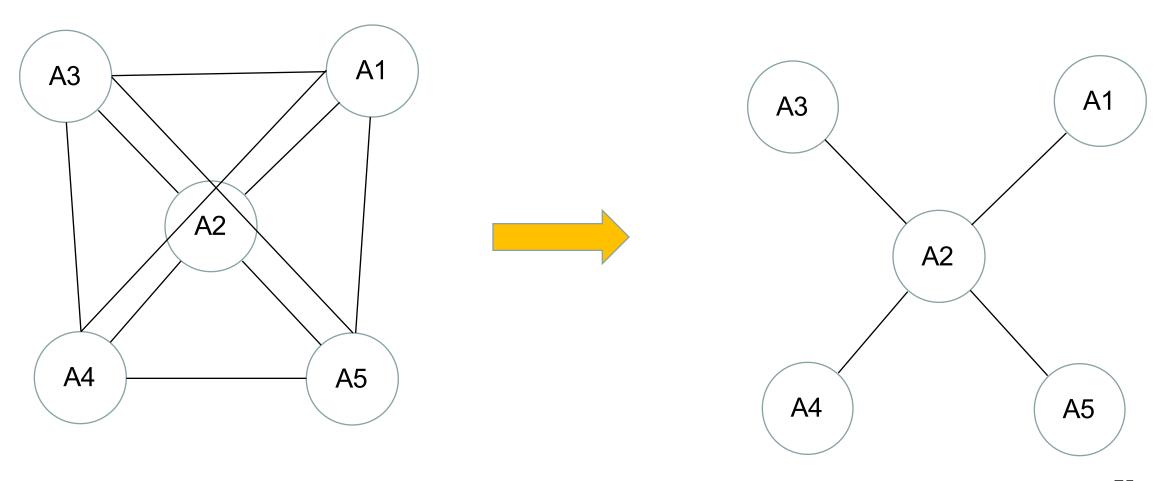
-0.3

**A5** 

 $Cor(A_1, A_3) \approx 1$ 



#### Motivation: Conditional independence is better



#### Motivation: Conditional independence is better

Conditional Independent

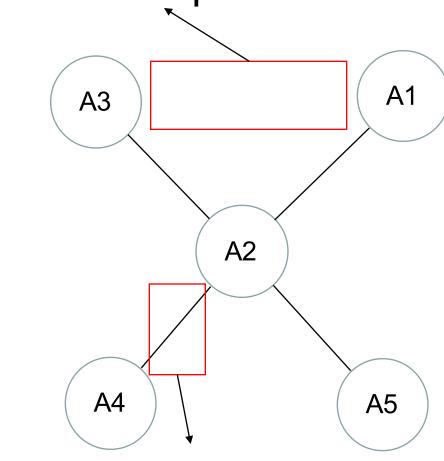
A1: Children are drown

A2: Weather is hot

A3: High sale of ice cream

A4: Wear less amount of clothes

A5: High Electricity Consumption



Conditional Dependent 76