A **Fast and Scalable** Joint Estimator for Integrating **Additional Knowledge** in Learning Multiple Related Sparse Gaussian Graphical Models

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http://jointggm.org/

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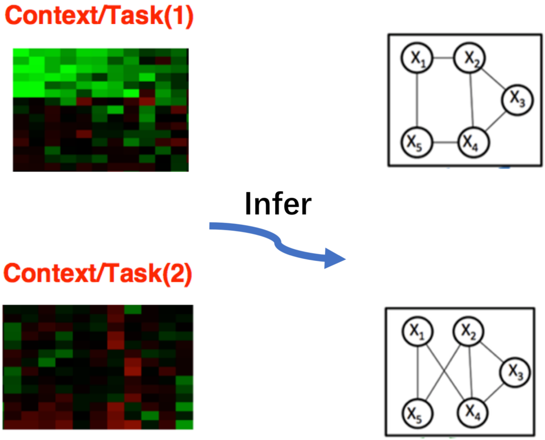
Motivation: Learning Multiple Related Graphs from Heterogeneous Samples about Multiple Contexts

- Multiple Datasets $\mathbf{X}^{(1)}, \ldots \mathbf{X}^{(K)}$ $\rightarrow$ Multiple Graphs $G^{(1)}, \ldots, G^{(K)}$.



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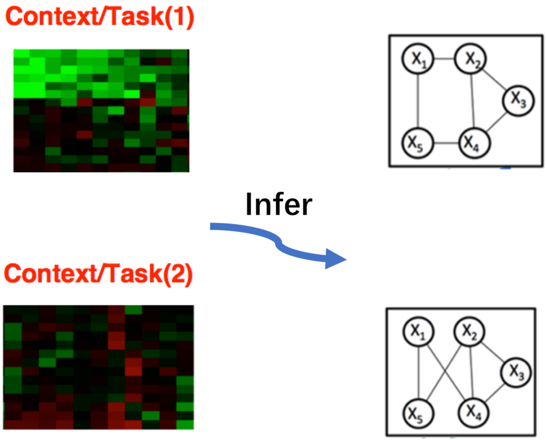

- e.g., Brain Connectomes from heterogeneous fMRI images
- e.g., Genetic Networks from heterogeneous RNA samples

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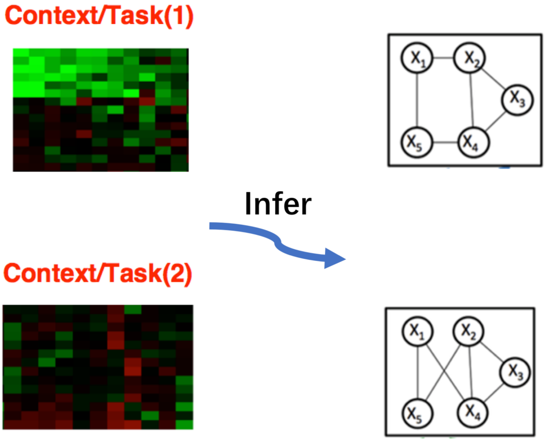
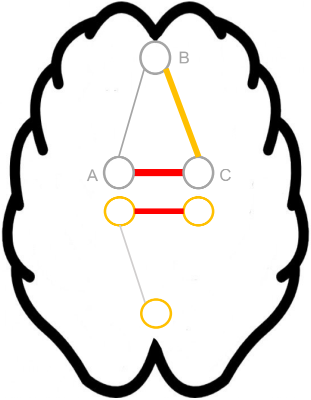


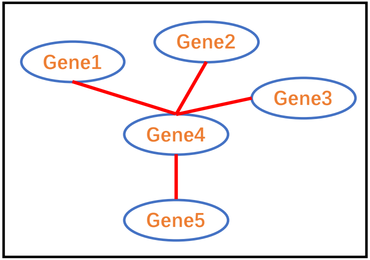
- Current Approch: Multi-sGGMs $\Rightarrow$ Multi-task sparse Gaussian Graphical Models

Limitation I: Missing Known Knowledge

- No clear ways to consider Known Additional Knowledge in multi-sGGMs.
- However, in real-world applications, plenty of known information. (e.g., red edges in the figures.)



Spatial Knowledge



Genetic Pathway

Limitation II: Slow computation and Not scalable

- K: number of tasks
  p: number of features

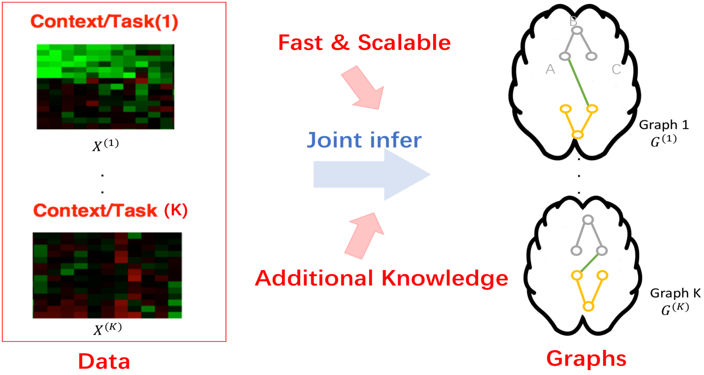
-

Method	Time Complexity	Bottleneck
W-SIMULE[1]	$O(K^4 p^5)$	LP with Kp variables
JGL[2]	$O(T \times Kp^3)$	SVD

[1] [Singh et al.(2017)Singh, Wang, and Qi]
[2] [Danaher et al.(2013)Danaher, Wang, and Witten]

Our Aim: Integrating Additional Knowledge in Scalable Learning of multi-sGGMs

- Our focus: How to estimate multiple graphs $G^{(1)}, \ldots, G^{(K)}$ from heterogeneous data $\mathbf{X}^{(1)}, \ldots \mathbf{X}^{(K)}$ and integrate additional knowledge.



Notations

$X^{(i)}$	i-th Data matrix.
$\Sigma^{(i)}$	i-th Covariance matrix.
$\Omega^{(i)}$	i-th Inverse of covariance matrix (precision matrix).
p	The total number of feature variables.
n_{tot}	The total number of samples.
X^{tot}	the concatenation of all Data matrices.
Σ^{tot}	the concatenation of all Covariance matrices.
Ω^{tot}	the concatenation of all Inverse of covariance matrices (precision matrices).
W_I^{tot}	$(W_I^{(1)}, W_I^{(2)}, \dots, W_I^{(K)})$
W_S^{tot}	$(W_S, W_S, \dots, W_S)$

Background: Elementary Estimator for sGGM

Elementary Estimator

$$\underset{\theta}{\operatorname{argmin}} \mathcal{R}(\theta)$$
$$\text{Subject to: } \mathcal{R}^*(\theta - \mathcal{B}^*(\widehat{\phi})) \leq \lambda_n \tag{1.1}$$

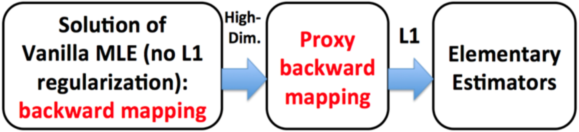
- For example, for sGGM:

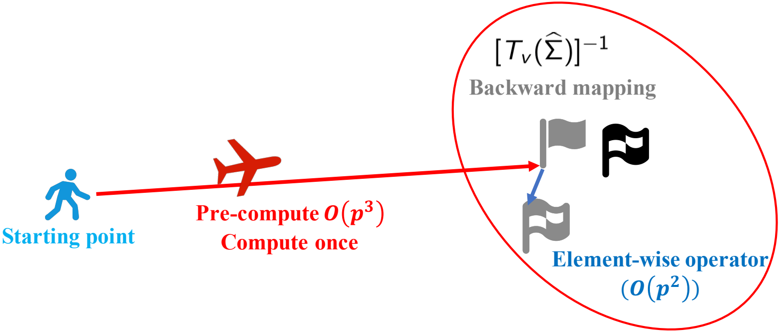
EE	$\mathcal{R}(\cdot)$	θ	$\mathcal{B}^*$	$\mathcal{R}^*$
EE-sGGM	$\|\cdot\|_1$	Ω	$[T_v(\widehat{\Sigma})]^{-1}$	$\|\cdot\|_\infty$

Elementary Estimator for sGGM

$$\underset{\Omega}{\operatorname{argmin}} ||\Omega||_1$$
$$\text{Subject to: } ||\Omega - [T_v(\widehat{\Sigma})]^{-1}||_\infty \leq \lambda_n \tag{1.2}$$

Background: Elementary Estimator – visualization





single-sGGM Method	Time Complexity	Note
QUIC[3]	$O(p^3)$	Not a closed-form solution
EE-sGGM[4]	$O(p^2)$	entry-wise closed-form sharp convergence rate

multi-sGGM Method	Time Complexity	Notes
W-SIMULE[5]	$O(K^4 p^5)$	LP with Kp variables
JGL[6]	$O(T \times Kp^3)$	SVD
Proposed method	$O(K^4 p^2)$	entry-wise fast sharp convergence rate

[3] [Hsieh et al.(2011)Hsieh, Sustik, Dhillon, and Ravikumar]
[4] [Yang et al.(2014)Yang, Lozano, and Ravikumar]
[5] [Singh et al.(2017)Singh, Wang, and Qi]
[6] [Danaher et al.(2013)Danaher, Wang, and Witten]

Proposed: Using Knowledge as Weight in Regularization (KW-norm)

- Integrating additional knowledge through a novel regularization function $\mathcal{R}(\cdot)$

KW-norm

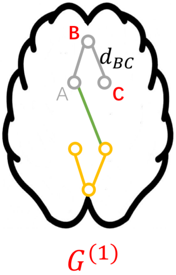
$$\mathcal{R}(\Omega^{tot}) = ||W_I^{tot} \circ \Omega_I^{tot}||_1 + ||W_S^{tot} \circ \Omega_S^{tot}||_1 \tag{2.1}$$

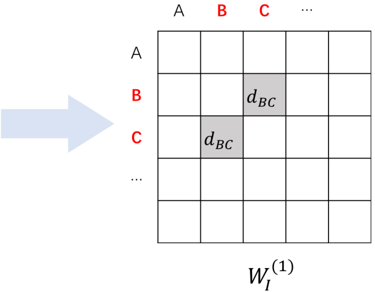
- W_I^{tot}: weights describing knowledge of each individual graph.
- W_S^{tot}: weights describing knowledge of the shared graph.

- KW-norm is flexible.

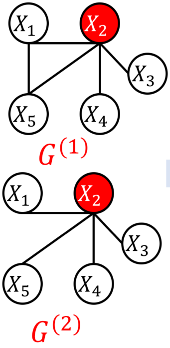
Example I: KW-norm representing the edge-level knowledge

- e.g., Spatial distance among brain regions;





- e.g., X_2 is a known hub node;



$$
\begin{array}{c|ccccc}
 & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & & 1/\gamma & 1 & 1 & 1 \\
2 & 1/\gamma & & 1/\gamma & 1/\gamma & 1/\gamma \\
3 & 1 & 1/\gamma & & 1 & 1 \\
4 & 1 & 1/\gamma & 1 & & 1 \\
5 & 1 & 1/\gamma & 1 & 1 &
\end{array}
$$

W_s

Proposed Method: Joint Elementary Estimator incorporating additional Knowledge (JEEK)

EE	$\mathcal{R}(\cdot)$	θ	$\mathcal{B}^*$	$\mathcal{R}^*$
EE-sGGM	$\|\| \cdot \|\|_1$	Ω	$[T_v(\widehat{\Sigma})]^{-1}$	$\|\| \cdot \|\|_\infty$
JEEK	kw-norm	Ω^{tot}	$inv[T_v(\widehat{\Sigma}^{tot})]$	kw-dual

JEEK

$$
\begin{aligned}
&\underset{\Omega_I^{tot},\Omega_S^{tot}}{\operatorname{argmin}} ||W_I^{tot} \circ \Omega_I^{tot}||_1 + ||W_S^{tot} \circ \Omega_S^{tot}|| \\
\text{Subject to: } & ||W_I^{tot} \circ (\Omega^{tot} - inv(T_v(\widehat{\Sigma}^{tot})))||_\infty \leq \lambda_n \\
& ||W_S^{tot} \circ (\Omega^{tot} - inv(T_v(\widehat{\Sigma}^{tot})))||_\infty \leq \lambda_n \\
& \Omega^{tot} = \Omega_S^{tot} + \Omega_I^{tot}
\end{aligned}
\tag{2.2}
$$

Proposed method: JEEK – Solution

- Fast and Scalable solution[7] – p^2 small linear programming subproblems:

$$\begin{aligned} &\underset{a_i, b}{\operatorname{argmin}} \sum_i |w_i a_i| + K|w_s b| \\ &\text{Subject to: } |a_i + b - c_i| \le \frac{\lambda_n}{\min(w_i, w_s)}, \\ &i = 1, \dots, K \end{aligned} \tag{2.3}$$

[7] $a_i := {\Omega_I^{(i)}}_{j,k}$ (the $\{j,k\}$-th entry of $\Omega^{(i)}$)
$b := {\Omega_S}_{j,k}$
$c_i = [T_v(\widehat{\Sigma}^{(i)})]^{-1}_{j,k}$.
$W^{(i)}_{j,k} = w_i$ and $W^S_{j,k} = w_s$.

Why JEEK is better

- Rich and flexible for integrating additional knowledge
    - e.g., spatial, anatomy, hub, pathway, location, known edges;

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- Parallelizable optimization with small sub-problems. Faster than the previous studies:

Method	Time Complexity	Additional Knowledge
JEEK	$O(K^4p^2)$ ($\Rightarrow$ $O(K^4)$ if parallelizing completely)	YES
W-SIMULE	$O(K^4p^5)$	YES
JGL	$O(T \times Kp^3)$	NO

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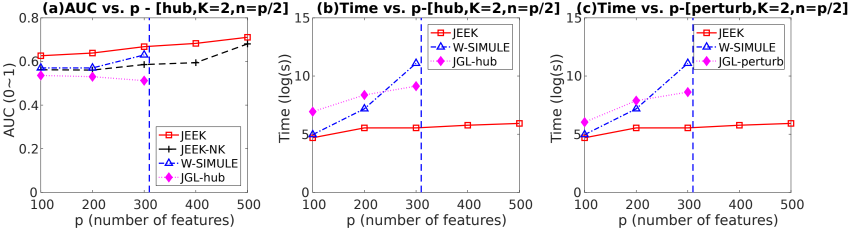
- Theoretical guaranteed

Theoretical Results

- Error bound: $||\Delta^* - \widehat{\Delta}||$
- Sharp convergence rate as the state-of-art

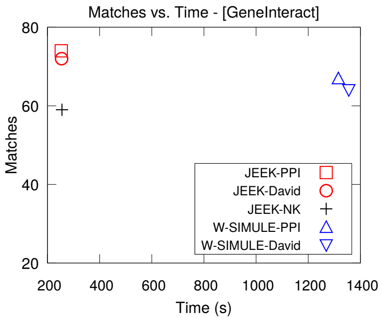
$$
\begin{aligned}
&||\widehat{\Omega}^{tot} - \Omega^{tot*}||_F \leq 4\sqrt{k_i + k_s}\lambda_n \\
&\max(||W_I^{tot} \circ (\widehat{\Omega}^{tot} - \Omega^{tot*})||_\infty, ||W_S^{tot} \circ (\widehat{\Omega}^{tot} - \Omega^{tot*}||_\infty) \leq 2\lambda_n \\
&||W_I^{tot} \circ (\widehat{\Omega}_I^{tot} - \Omega_I^{tot*})||_1 + ||W_S^{tot} \circ (\widehat{\Omega}_S^{tot} - \Omega_S^{tot*})||_1 \leq 8(k_i + k_s)\lambda_n
\end{aligned} \tag{3.1}
$$

Empirical Results on Multiple Synthetic Datasets

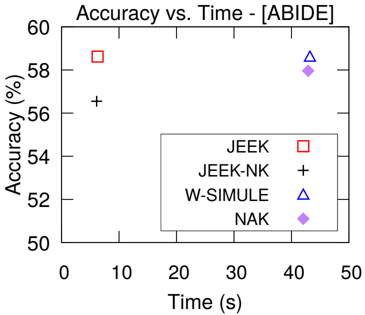


- JEEK outperforms the speed of the state-of arts significantly;
- JEEK obtains better or same AUC as the state-of-the-art;
- JEEK obtains better AUC than JEEK-NK (no additional knowledge).

Empirical Results on Two Real-world Datasets



(a)



(b)

- (a). On real-world gene expression data about leukemia cells vs. normal blood cells. Used multiple types of additional knowledge;
- (b). On real-world Brain fMRI dataset: ABIDE. Using LDA as a downstream classification for evaluating JEEK vs. baselines.

R Package Publicly Available !!!

- The project website: `http://jointggm.org/`
- R package "jeek":
  - `install.packages("jeek")`
  - `library("jeek")`
  - `demo(jeek)`

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