

JOINT ESTIMATION OF MULTIPLE GRANGER GRAPHICAL MODELS USING NON-CONVEX PENALTIES

Thesis Proposal

Parinthorn Manomaisaowapak

Advisor: Assist. Prof. Dr. Jitkomut Songsiri

Department of Electrical Engineering, Faculty of Engineering

Chulalongkorn University

OUTLINE

- Introduction
- Overview
- Related works
- Work plan
- Background
- Methodology
- Preliminary results
- Future works

INTRODUCTION

How to study relationship of variables?

Causality analysis

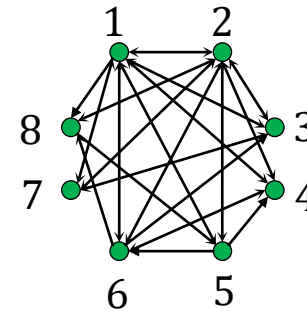
A strength of evidence

Granger causality(GC)

- Based on dynamical models
- Directly related to sparsity of model coefficient

Graphical representation

Causality network



Causality matrix

	1	2	3	4	5	6	7	8
1	Black	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow
2	Yellow	Black	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow
3	Yellow	Yellow	Black	Yellow	Yellow	Yellow	Yellow	Yellow
4	Yellow	Yellow	Yellow	Black	Yellow	Yellow	Yellow	Yellow
5	Yellow	Yellow	Yellow	Yellow	Black	Yellow	Yellow	Yellow
6	Yellow	Yellow	Yellow	Yellow	Yellow	Black	Yellow	Yellow
7	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Black	Yellow
8	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Black

Granger graphical model

INTRODUCTION

High dimensional GC network

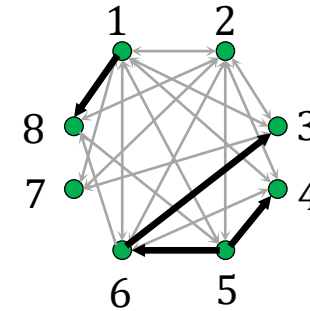
- GC network has **large amount of connections**
- We aim to extract only **significant connections**



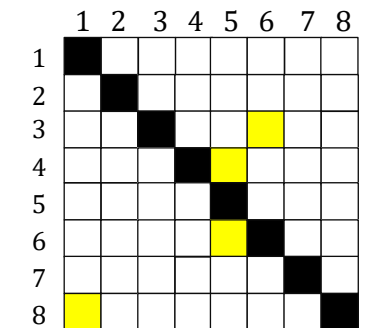
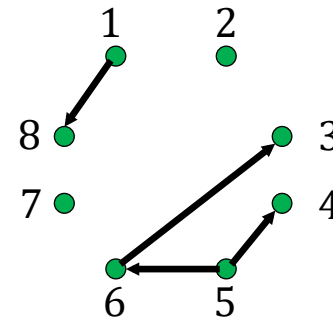
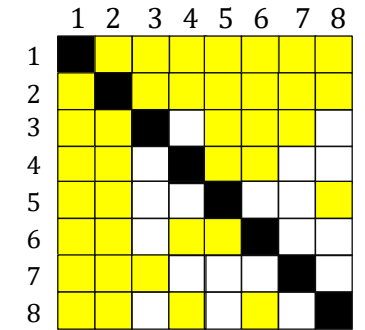
Sparse representation of GC network

Graphical representation

Causality network



Causality matrix



INTRODUCTION

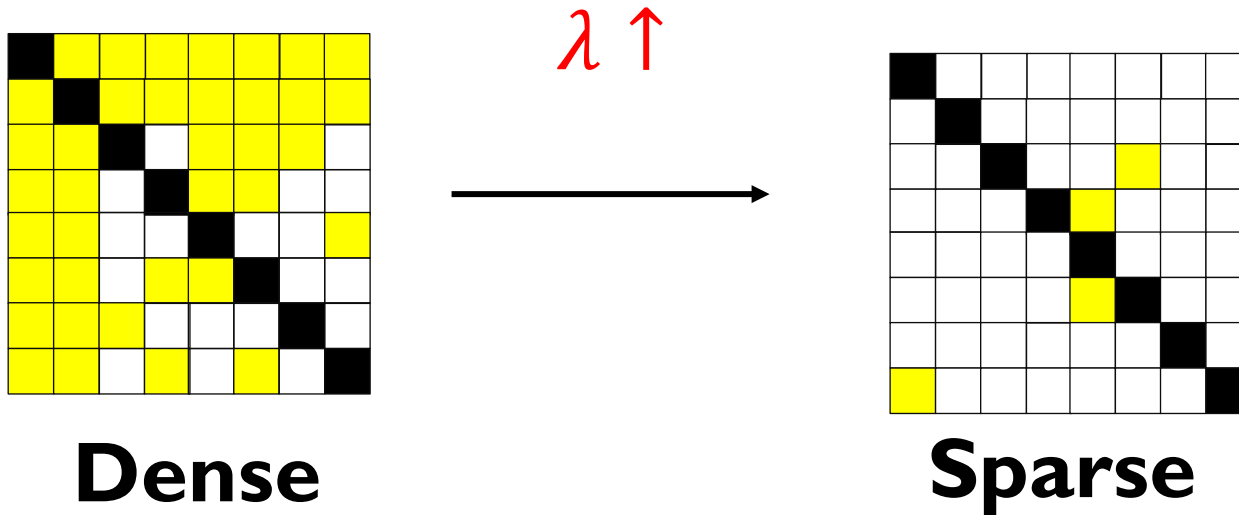
Sparse estimation formulation in general form.

$$\min_{\theta} f(\theta) + \lambda g(\theta)$$

Model parameter

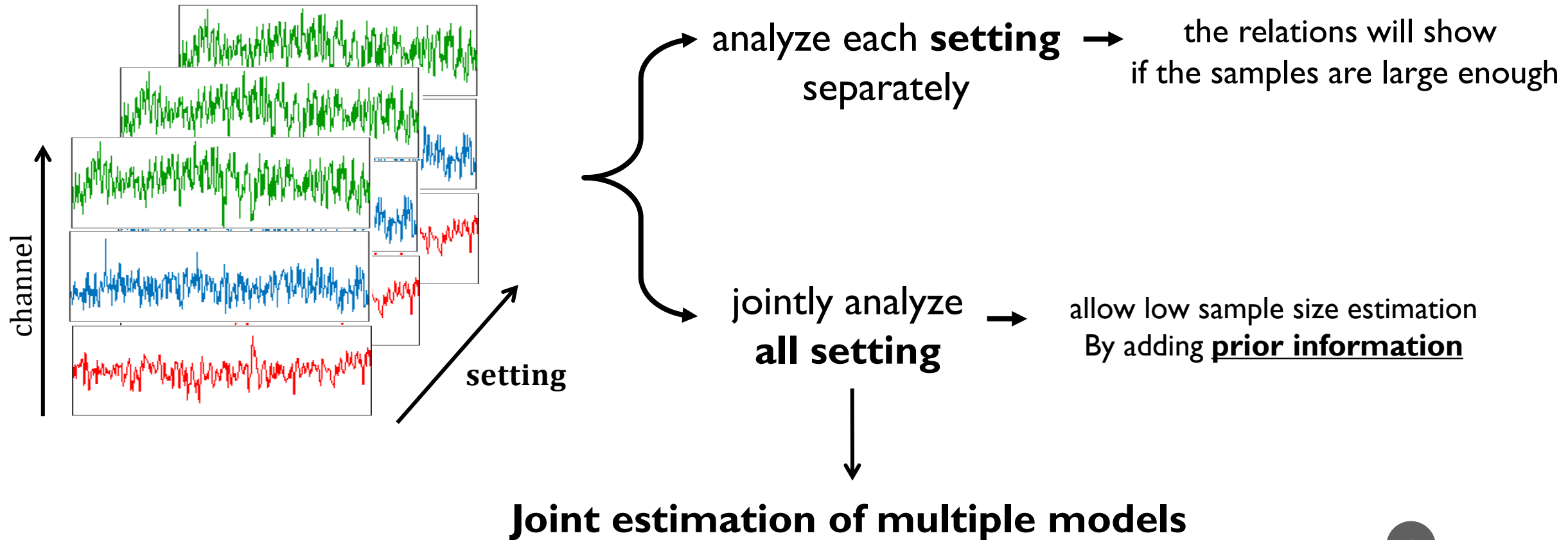
Fitting term

Sparsity inducing penalty



INTRODUCTION

consider when the same multivariate time-series are measured in different settings



INTRODUCTION

Goal: Find important connections of multiple networks with prior knowledge

$$\min_{\theta_1, \dots, \theta_K} \sum_i [f_i(\theta_i) + \lambda_1 h_i(\theta_i)] + \lambda_2 g(\theta_1, \dots, \theta_K)$$

where h_i aims to promote differential sparsity in each model. ●

g aims to promote common sparsity across all models. ●

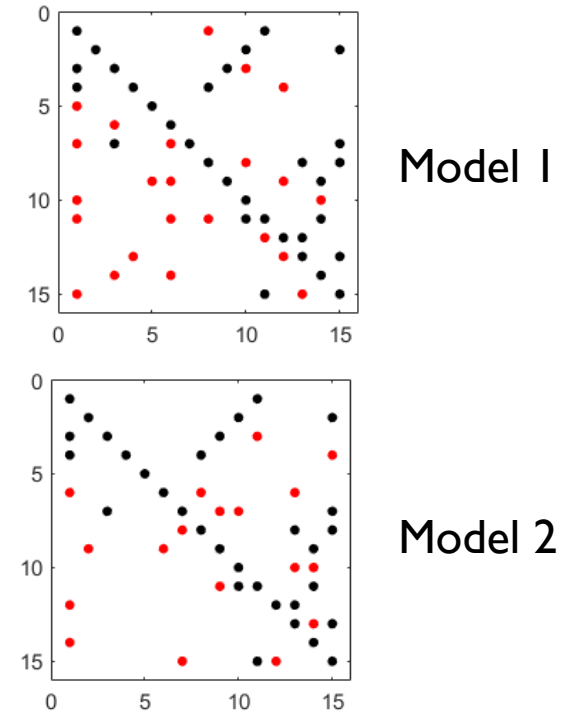
Require **definition of similarity**

→ Sparsity inducing function

Example

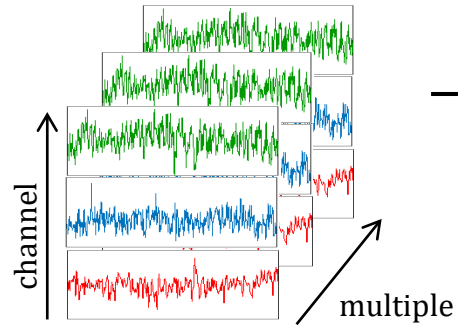
group lasso → $\theta_1, \dots, \theta_K$ has **same non-zero pattern**

fused lasso → $\theta_m - \theta_\ell$ is sparse → **Some model coefficients are identical**

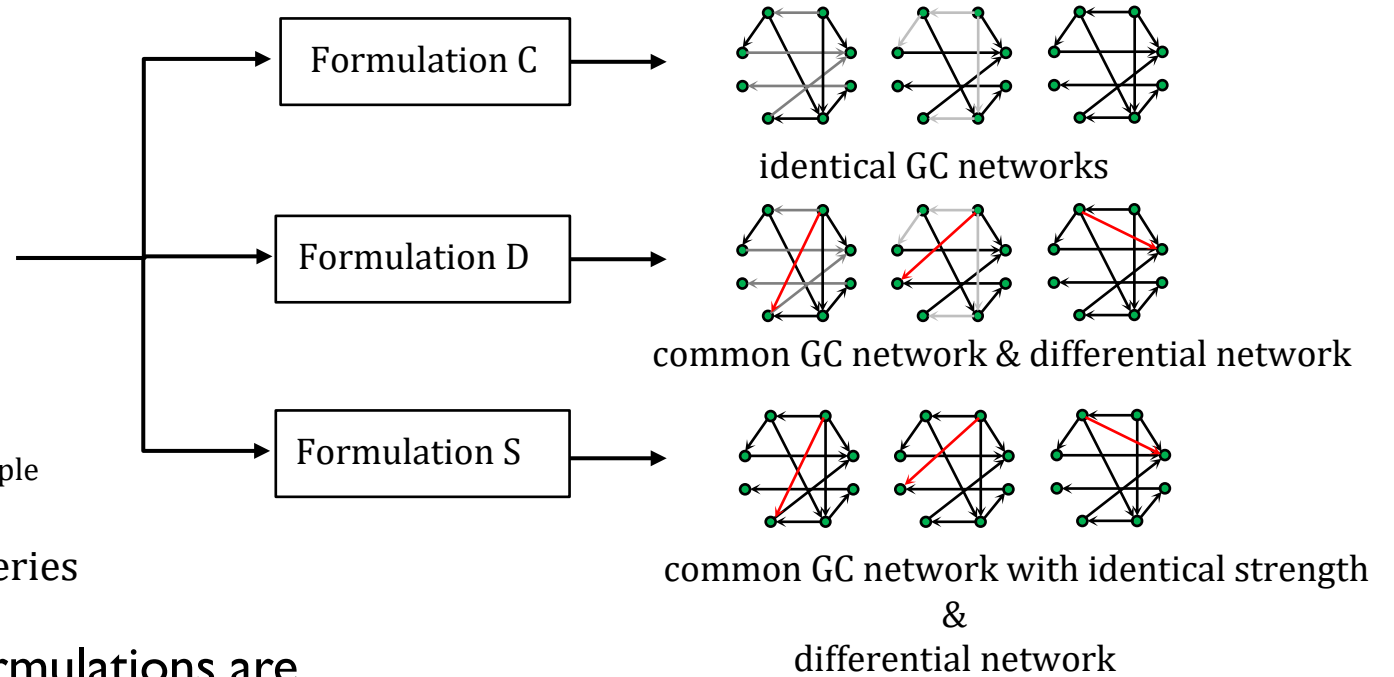


THESIS OVERVIEW

Objectives



Multiple multivariate time-series



- To propose three formulations. The formulations are
 - Formulation C: The estimated networks have an **identical sparsity pattern**
 - Formulation D: The estimated networks have some common parts and some different parts.
 - Formulation S: The estimated networks have some common parts and some different parts. The common parts also **share model parameters**.
- To provide efficient numerical methods for solving the proposed estimation methods in a large-scale setting.

Scope of work

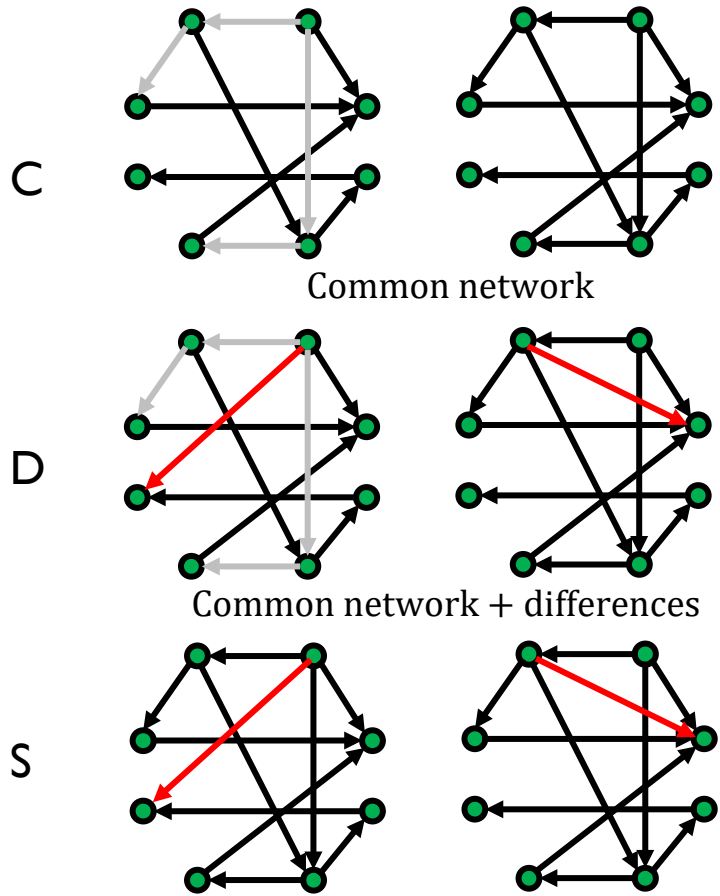
- The proposed framework will be verified intensively in a simulated data sets and one real-world data set
- The usefulness of the methods will be illustrated on brain network application

Expected outcome

- Estimation formulations of multiple Granger graphical models
- A computer program that has input as a set of multivariate time-series and return group and individual Granger graphical model of the multiple time-series

RELATED WORKS

non-convex group penalties [Our work]



Common network has identical strength + differences

[Songsiri, 2017]

group lasso, fused lasso

[Wilms, 18]
[Gregorova, 2015]

group lasso
group lasso+Tikhonov

[Skripnikov, 2019]
[Guo, 2011],
[Chun, 2015]

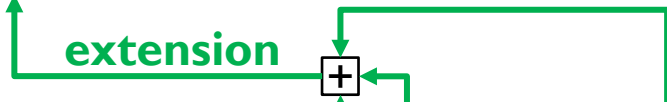
group lasso, two-stages
non-convex penalty
Gaussian graphical model

[Skripnikov, 2019]
[Tuck, 2020]

sparse fused-lasso
sparse fused-lasso
Gaussian graphical model

[Bore, 2020]

non-convex penalty
single Granger model



non-convex group norm penalty
 $\sum \|x_{G_i}\|_p^q \quad p \geq 1, 0 < q < 1$

[Hu, 2017]

non-convex penalty
 $\sum |x_i|^q \quad 0 < q < 1$

[Chartrand, 2008]

WORK PLAN

Literature survey

- Joint estimation
 - Gaussian graphical models
 - Granger graphical models
- Numerical methods
 - Convex optimization
 - Non-convex optimization



Problem formulation

Convex & non-convex penalties

- Formulation **C** —————→
 - Identical sparsity pattern GC networks
- Formulation **D** —————→
 - Common network pattern with differences
- Formulation **S** —————→
 - Identical VAR coefficients with differences

Implementation

convex	non-convex
C	C
D	D
S	S

Experiments

- Algorithm hyperparameters selection and testing
- Efficiency evaluation of numerical methods
- Effectiveness of formulations
- Brain network application



Thesis writing & Publications

BACKGROUND

Vector autoregressive model (VAR)

$$y(t) = \sum_{r=1}^p A_r y(t-r) + \eta(t)$$

$$A_r \in \mathbf{R}^{n \times n} \quad y = (y_1, \dots, y_n) \in \mathbf{R}^n$$

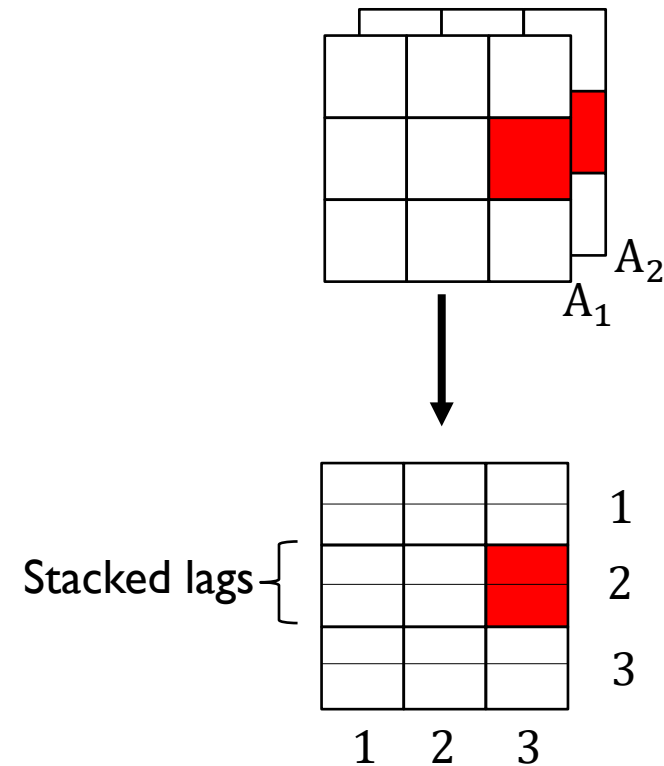
Granger causality on VAR models

- Granger causality (GC, F_{ij}) is a strength of evidence
- Absence of GC connection can be investigated by the relation

$$F_{ij} = 0 \Leftrightarrow (A_r)_{ij} = 0; r = 1, 2, \dots, p \quad [\text{Granger, 1980}]$$

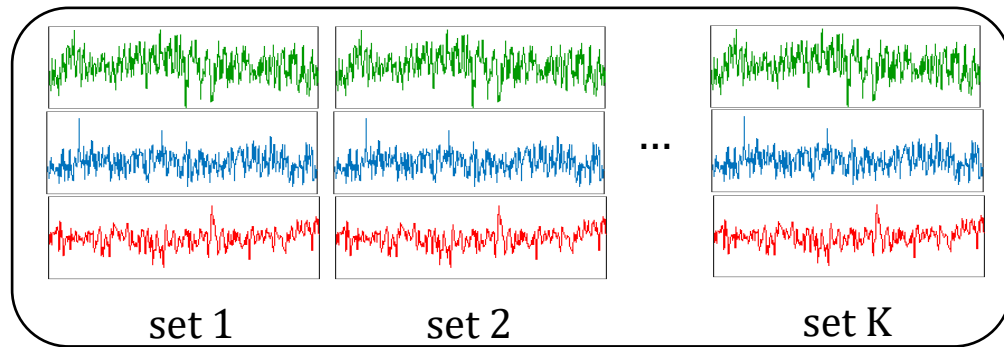


Sparsity inducing penalty can be designed using this prior knowledge



METHODOLOGY

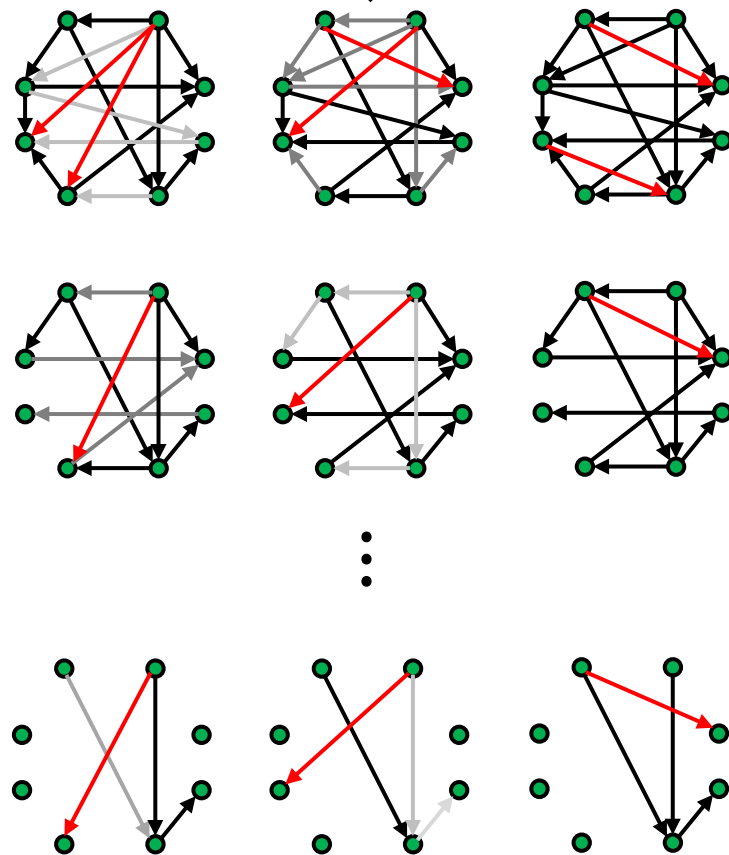
OVERVIEW



K multivariate time-series

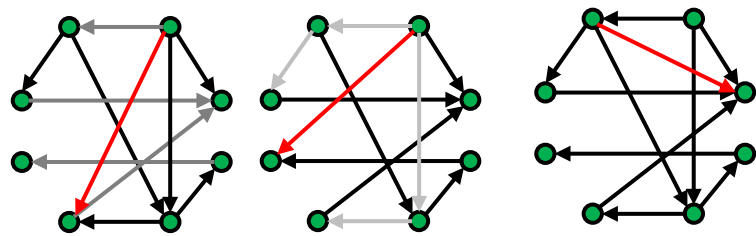


Joint estimation formulation



vary sparsity

Model selection



Estimated networks

We proposed three formulations,

Formulation **C** **Common**

- Common pattern.

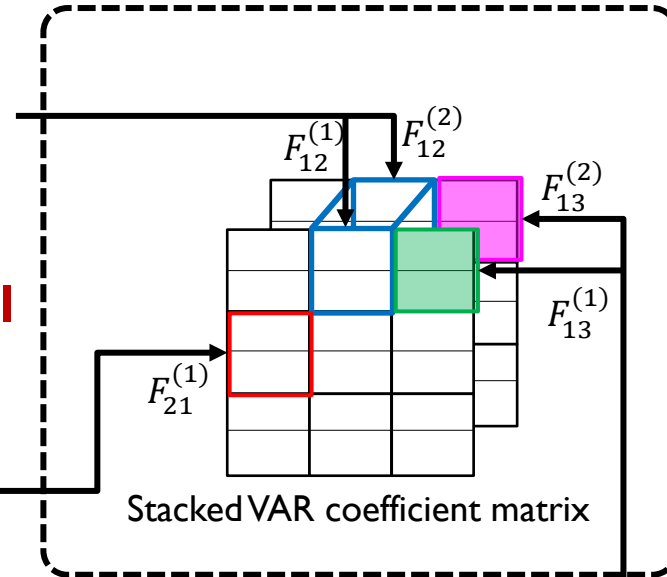
Formulation **D** **Differential**

- Common pattern
- Different pattern

Formulation **S** **Similar**

- Shared VAR coefficients value in all models
- Different pattern

Induce block sparsity by group norm penalty



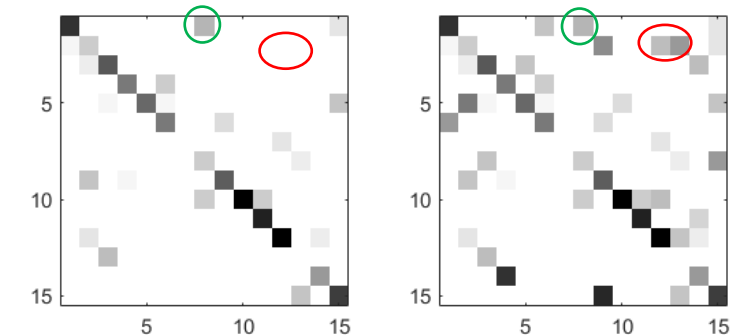
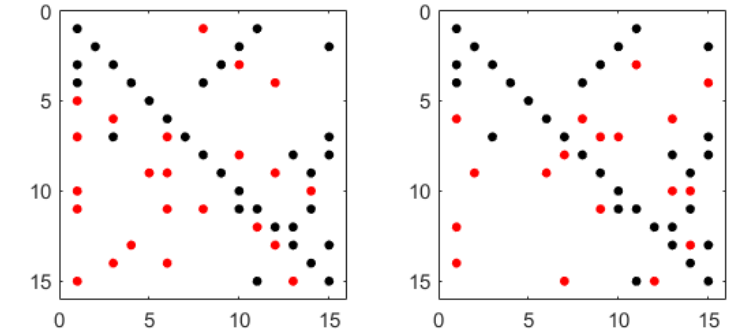
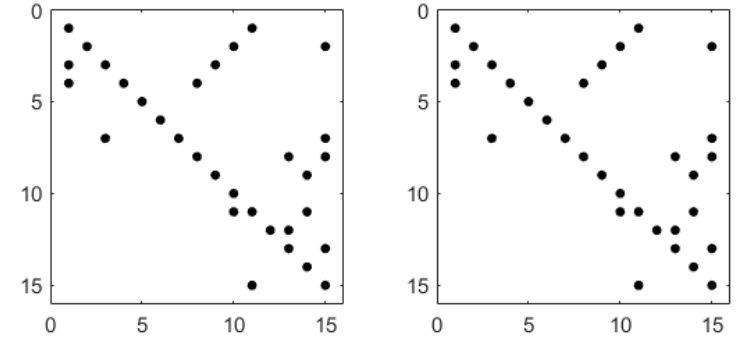
Stacked VAR coefficient matrix

C

D

S

Expected outcome



Model 1

Model 2

We used BIC criteria to find **optimal tuning-parameters**

$$BIC(\lambda_1, \lambda_2) = -2 \mathcal{L}(\lambda_1, \lambda_2) + \log(N) \cdot df(\lambda_1, \lambda_2)$$

Log-likelihood of VAR model.
(Fitness of models)

Effective degree of freedom
(Complexity of models).

off-diagonal **nonzero** estimated parameters

There are other choices.

Problem properties (Formulation C, D, S)

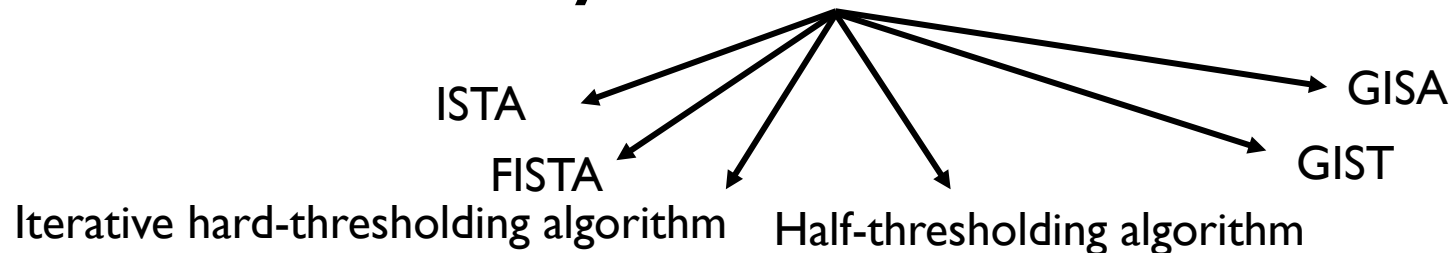
- The problem is in the form of $\min_x f(x) + g(x)$
- ∇f is Lipschitz-continuous.
- Function g is not differentiable at zero while we prefer sparse solutions
- We aim to solve high-dimensional problem or in a large-scale setting.



First order algorithm should be considered first



Proximal gradient methods unify the framework that solve this problem



Proximal algorithms

- require evaluation of **proximal operator**

Definition: proximal operator of function g

$$\text{prox}_{\alpha g}(v) = \underset{x}{\text{argmin}} \ g(x) + \frac{1}{2\alpha} \|x - v\|_2^2$$

- are widely used in sparse estimation using lasso, group lasso for a convex case
- proximal operator has a closed-form expression for some functions, such as

$$\ell_1 \text{ norm} \quad (\text{prox}_{\lambda \|x\|_1}(v))_i = \text{sign}(v_i) \max\{0, v_i - \lambda\}$$

Soft thresholding operator

$$\ell_2 \text{ norm} \quad \text{prox}_{\lambda \|x\|_2}(v) = \max\left\{0, 1 - \frac{\lambda}{\|v\|_2}\right\} v$$

Block-soft thresholding operator

METHODOLOGY

ALGORITHM

its special case is FISTA

proximal gradient algorithm

Solve $\min_x F(x) = f(x) + g(x)$



$$x^+ = \text{prox}_{\alpha g}(x - \alpha \nabla f(x))$$



Have a sufficient descent property in F



**Globally converge for our formulation
in non-convex setting**
by virtue from its sufficient descent property

But it is slow

accelerated proximal gradient(APG)

- $y = x^- + \text{correction term}$
- $x^+ = \text{prox}_{\alpha g}(y - \alpha \nabla f(y))$
- update correction term

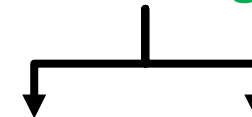
not a sufficient descent method



no convergence guaranteed for our formulation



add a monitoring scheme [Li, 2015]



monotone APG

non-monotone APG



Globally converges in our formulations

METHODOLOGY

ALGORITHM

proximal gradient methods

solve $\min_x F(x) = f(x) + g(x)$



require proximal operator of $g(x) = h_1(L_1x) + h_2(L_2x)$



only $h_1(x), h_2(x)$ have closed-form proximal operator [Hu, 2017]

Alternating direction methods of multipliers(ADMM)

solve $\min_{x,z} F(x) = f(x) + g(z) + \rho \|Ax + Bz - c\|_2^2$
subjected to $Ax + Bz = c$



set $A = \begin{bmatrix} L_1 \\ L_2 \end{bmatrix}, B = -I, c = 0$



Evaluation of $\text{prox}_{\alpha g}(v)$
Reduce to $\text{prox}_{\alpha h_1}(v), \text{prox}_{\alpha h_2}(v)$



no convergence guaranteed in non-convex formulations



a convergence to critical point can be obtained by selecting a proper penalty parameter ρ

related work: **SDMM** [Combettes, 2011]

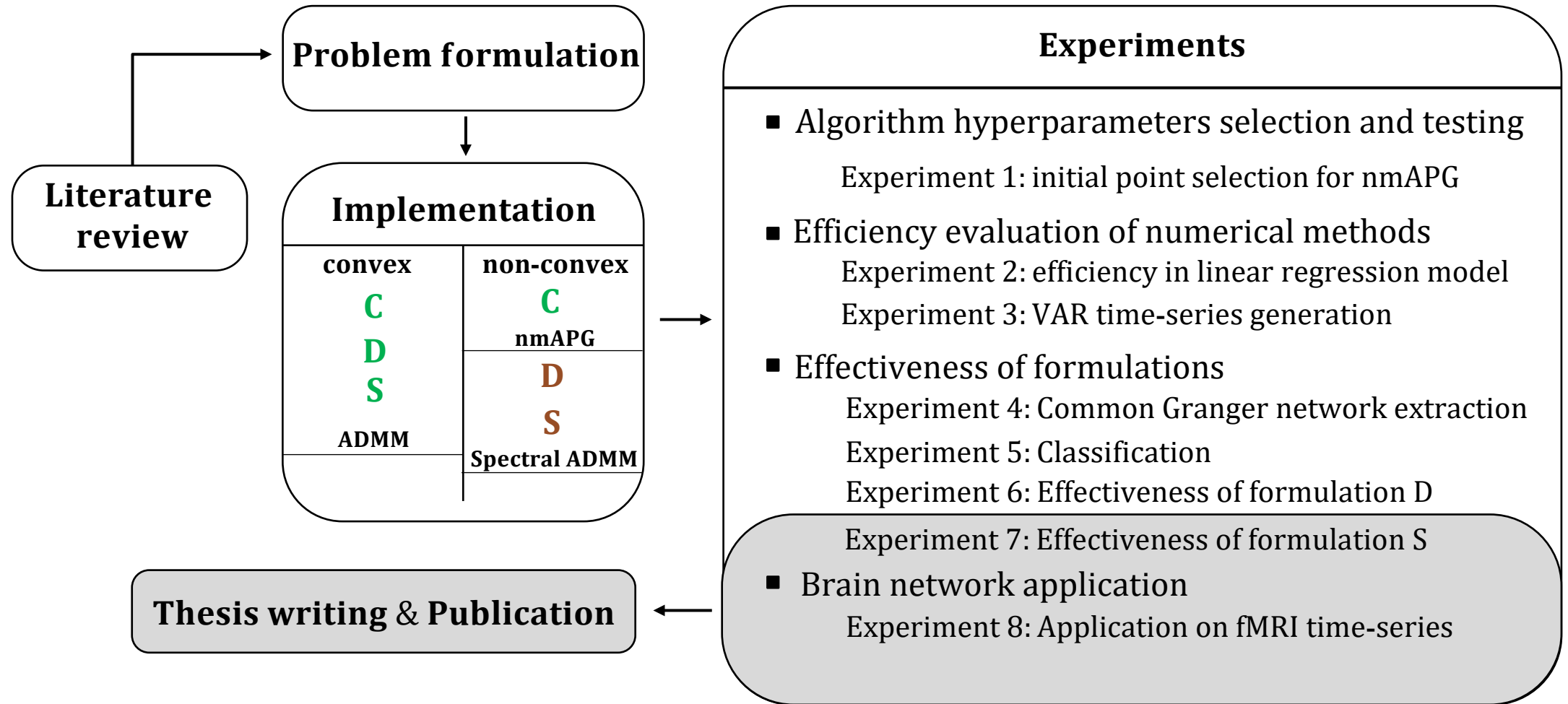
set $A = \begin{bmatrix} I \\ L_1 \\ L_2 \end{bmatrix}, B = -I, c = 0$



Higher computation complexity than ours

adaptive ρ may solve the problem → Spectral ADMM [Xu, 2017]

PRELIMINARY RESULTS



PRELIMINARY RESULTS

Performance index

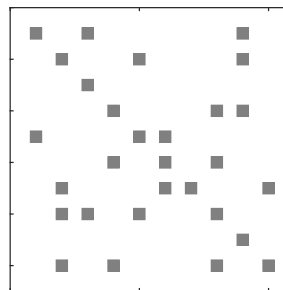
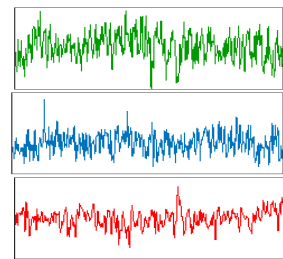
- Area under ROC curve

$$\text{FPR} = \frac{\text{False positive}}{\# \text{ Negative}}$$

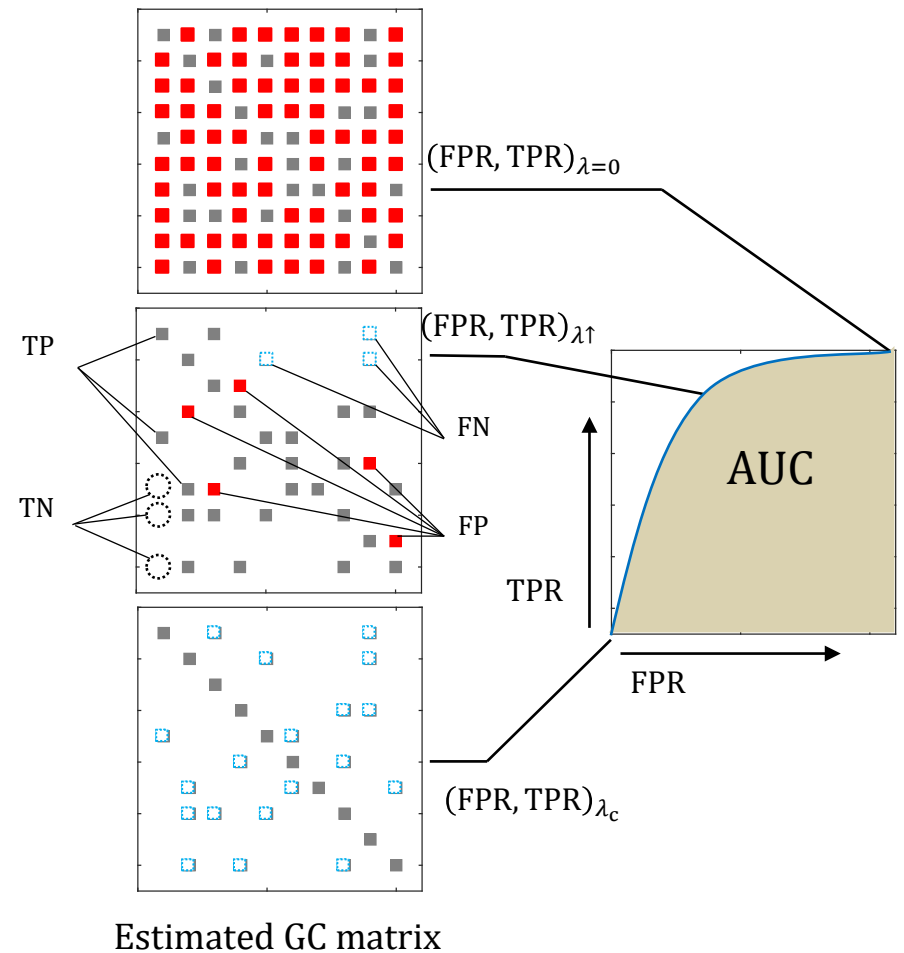
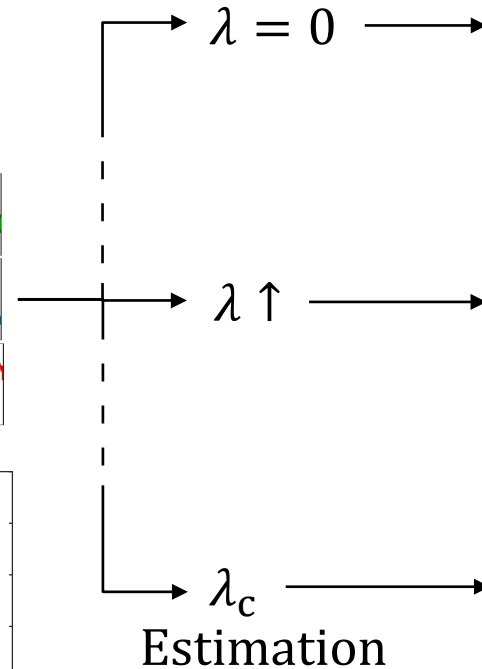
$$\text{TPR} = \frac{\text{True positive}}{\# \text{ Positive}}$$

- Relative parameter bias

$$\frac{\|\hat{x} - x_{\text{true}}\|_2}{\|x_{\text{true}}\|_2}$$



Ground-truth



PRELIMINARY RESULTS

Experiment 3: VAR time-series with prespecified GC patterns generation

Objective: To test the formulations with known given structure

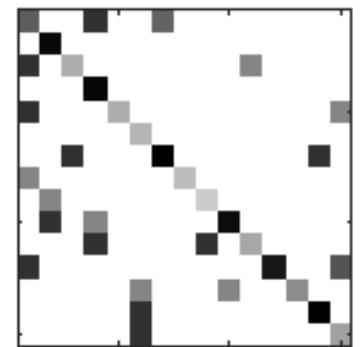
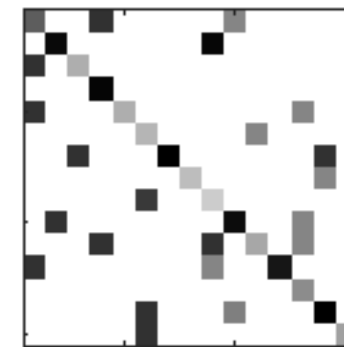
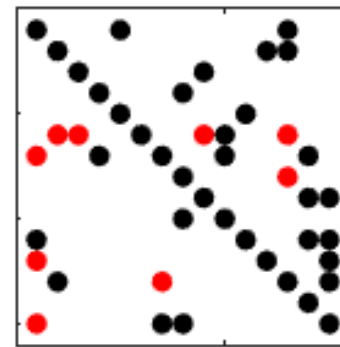
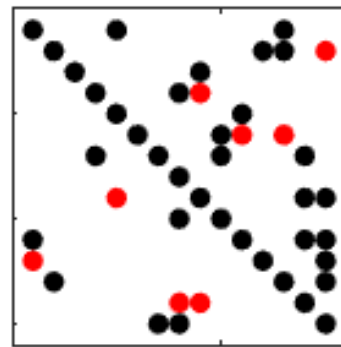
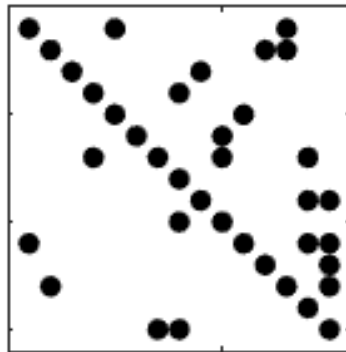
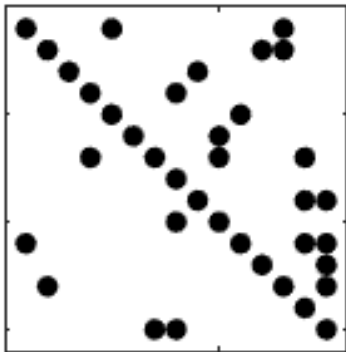
We randomized **stable VAR coefficients** that the Granger causality patterns are

1. **Common type** ground truth

2. **Differential type** ground truth

3. **Similar type** ground truth

Examples of generated GC matrix topology

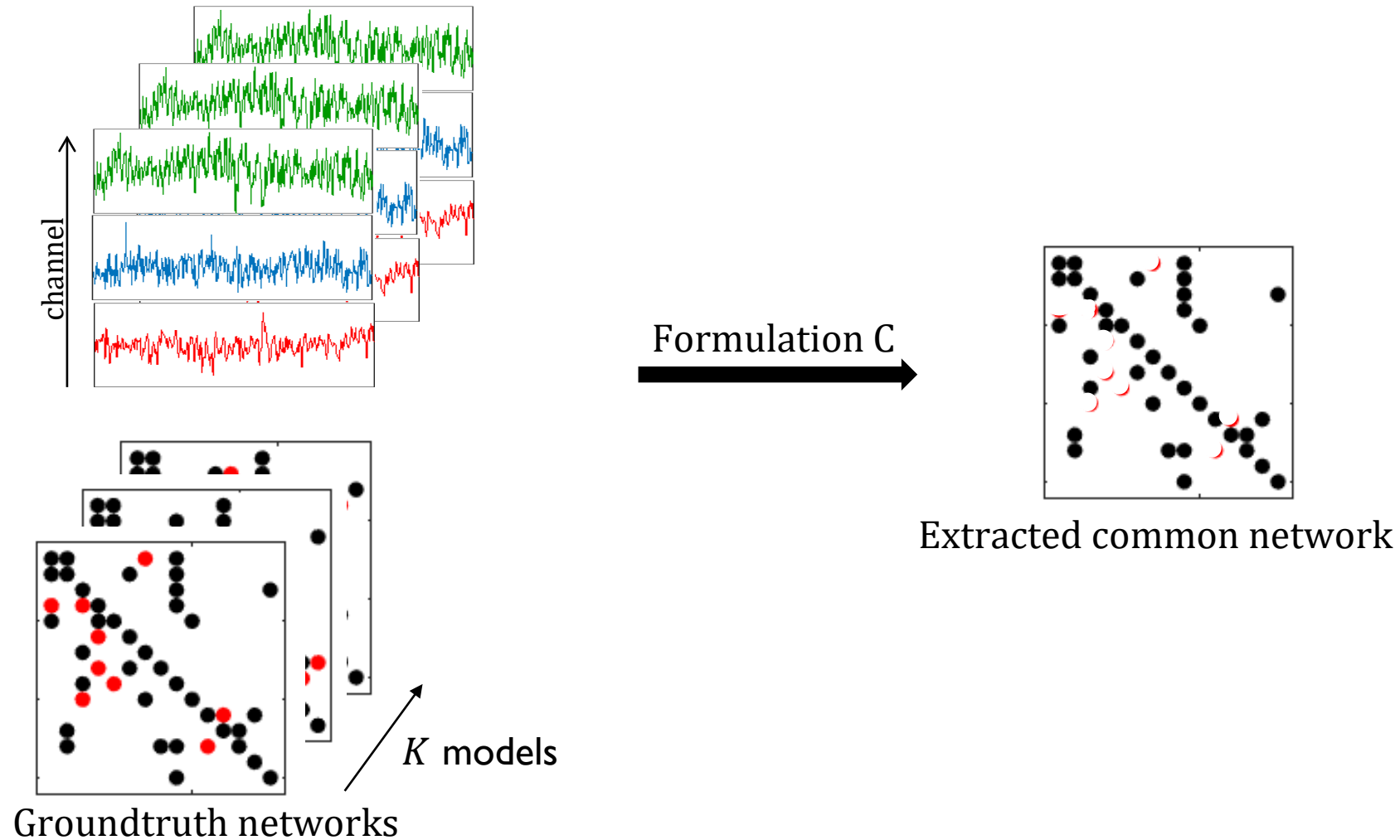


Common network density and **differential network** density can be set.

PRELIMINARY RESULTS

Experiment 4: Group level Granger network extraction

Objective: To extract common GC network with a presence of heterogeneous connections

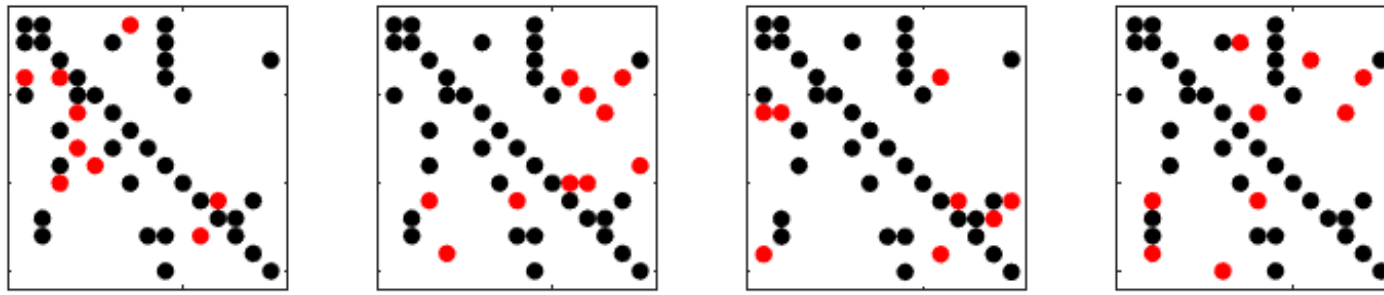


PRELIMINARY RESULTS

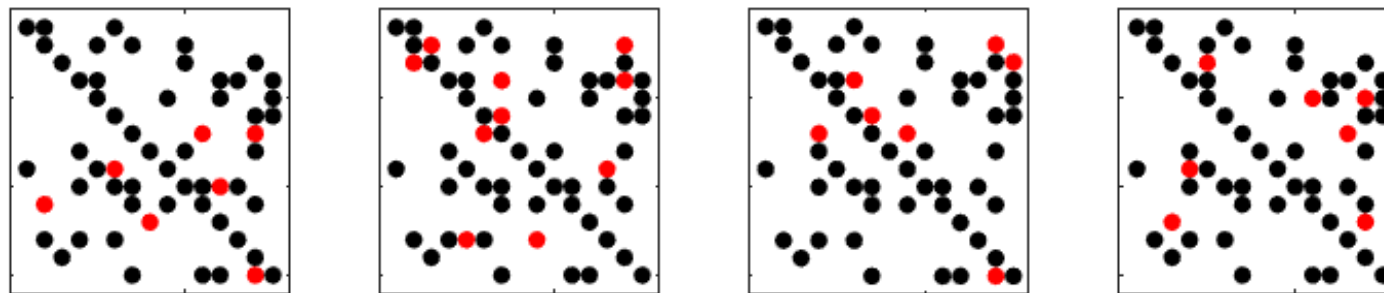
Experiment 4: Group level Granger network extraction

Objective: To extract common GC network with a presence of heterogeneous connections

- 4 sets of 15-dimensional 2nd-order-VAR models
- Common density : 10%, 20%
- Differential density : 5%



Common density = 10%



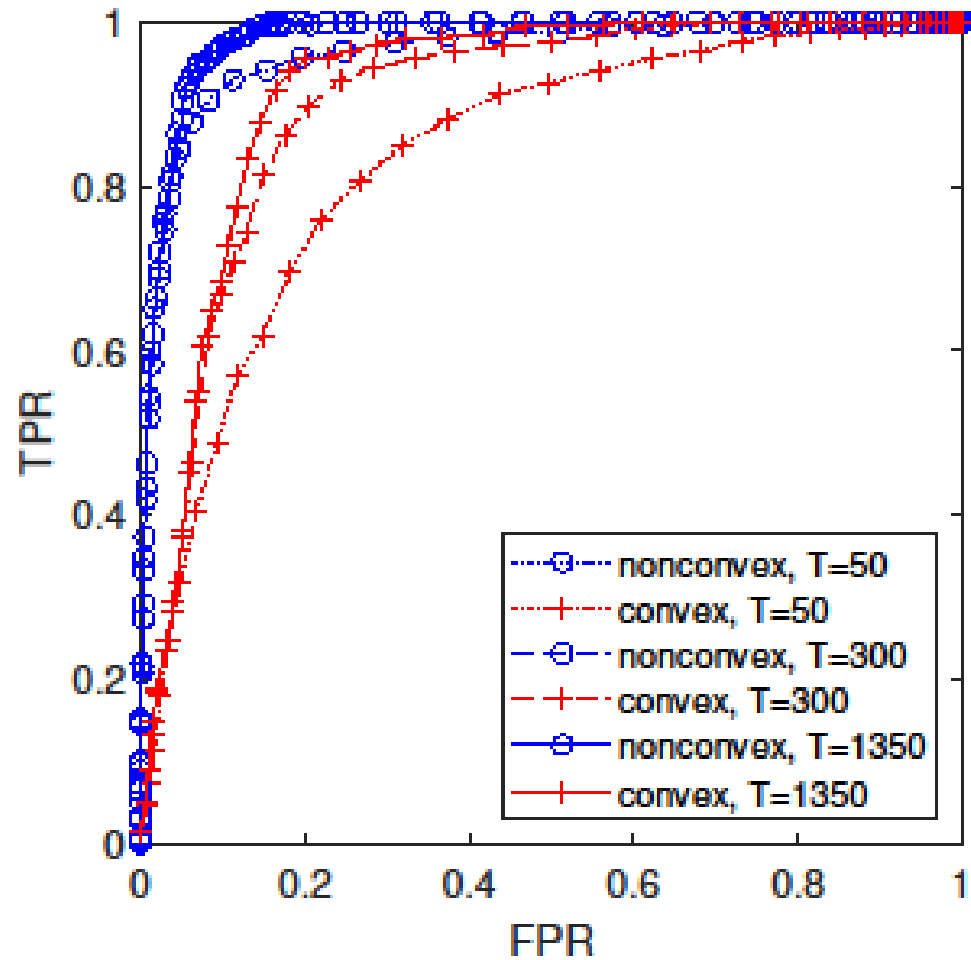
Common density = 20%



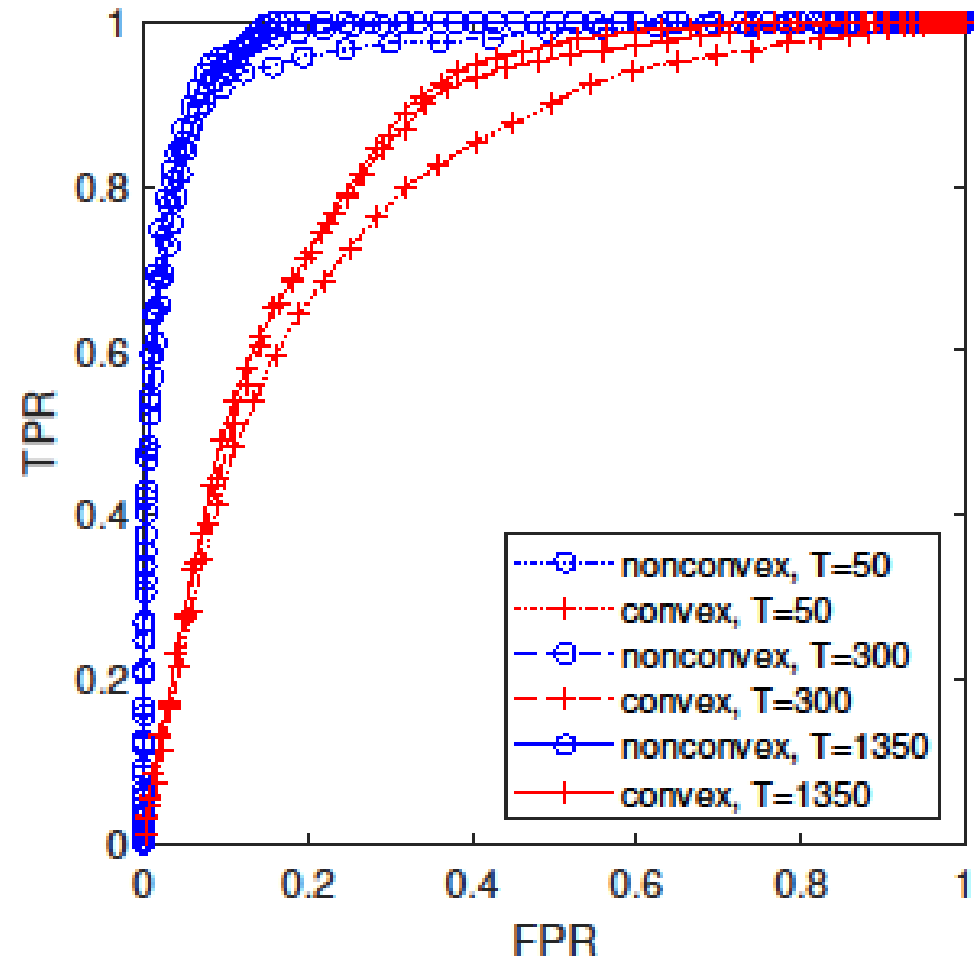
Generate time-series with unit variance Gaussian noise.

PRELIMINARY RESULTS

Experiment 4: Group level Granger network extraction



Common density : 0.1

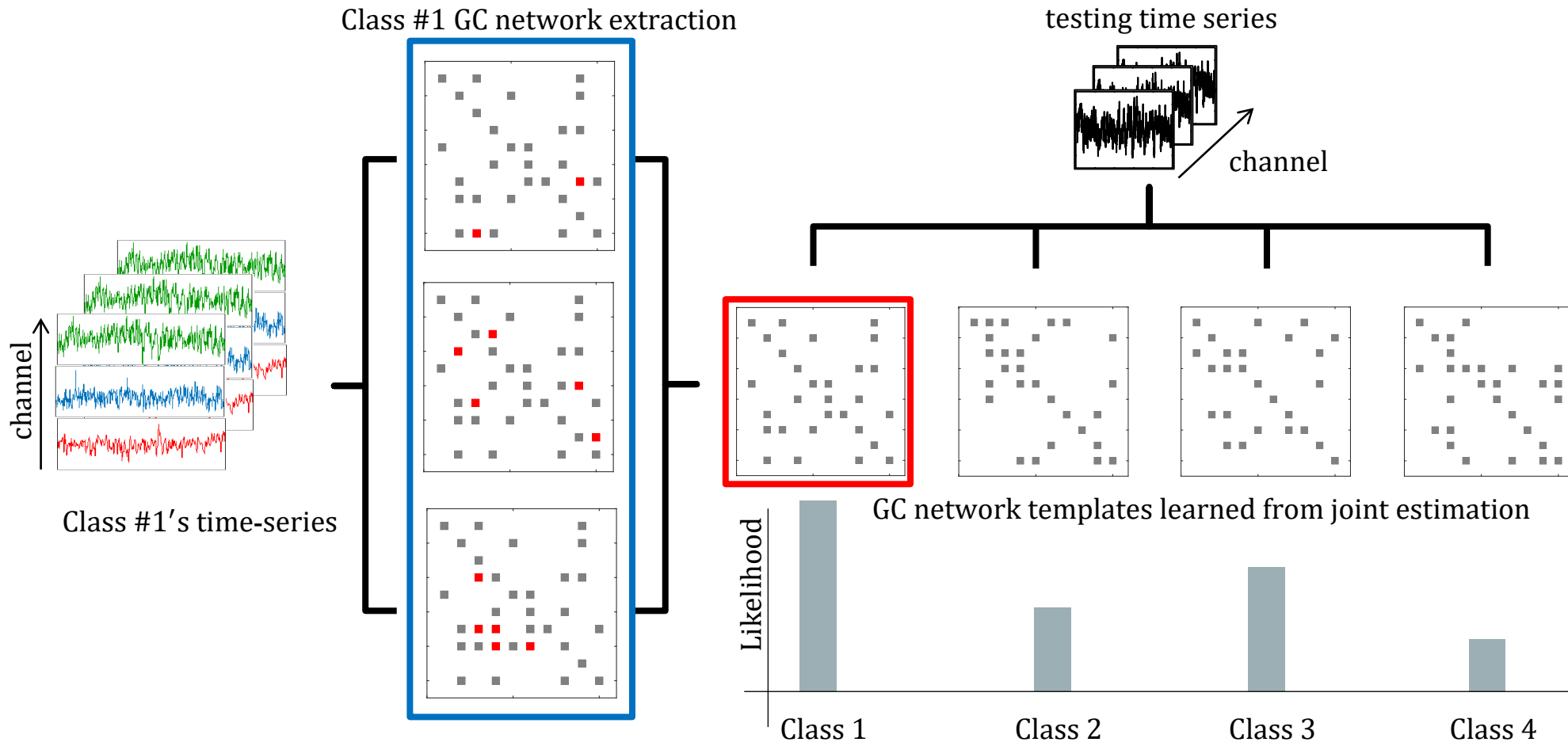


Common density : 0.2

PRELIMINARY RESULTS

Experiment 5: Supervised-classification using learned common Granger network

Objective: To illustrate the application of common Granger network extraction



PRELIMINARY RESULTS

Experiment 5: Supervised-classification using learned common Granger network

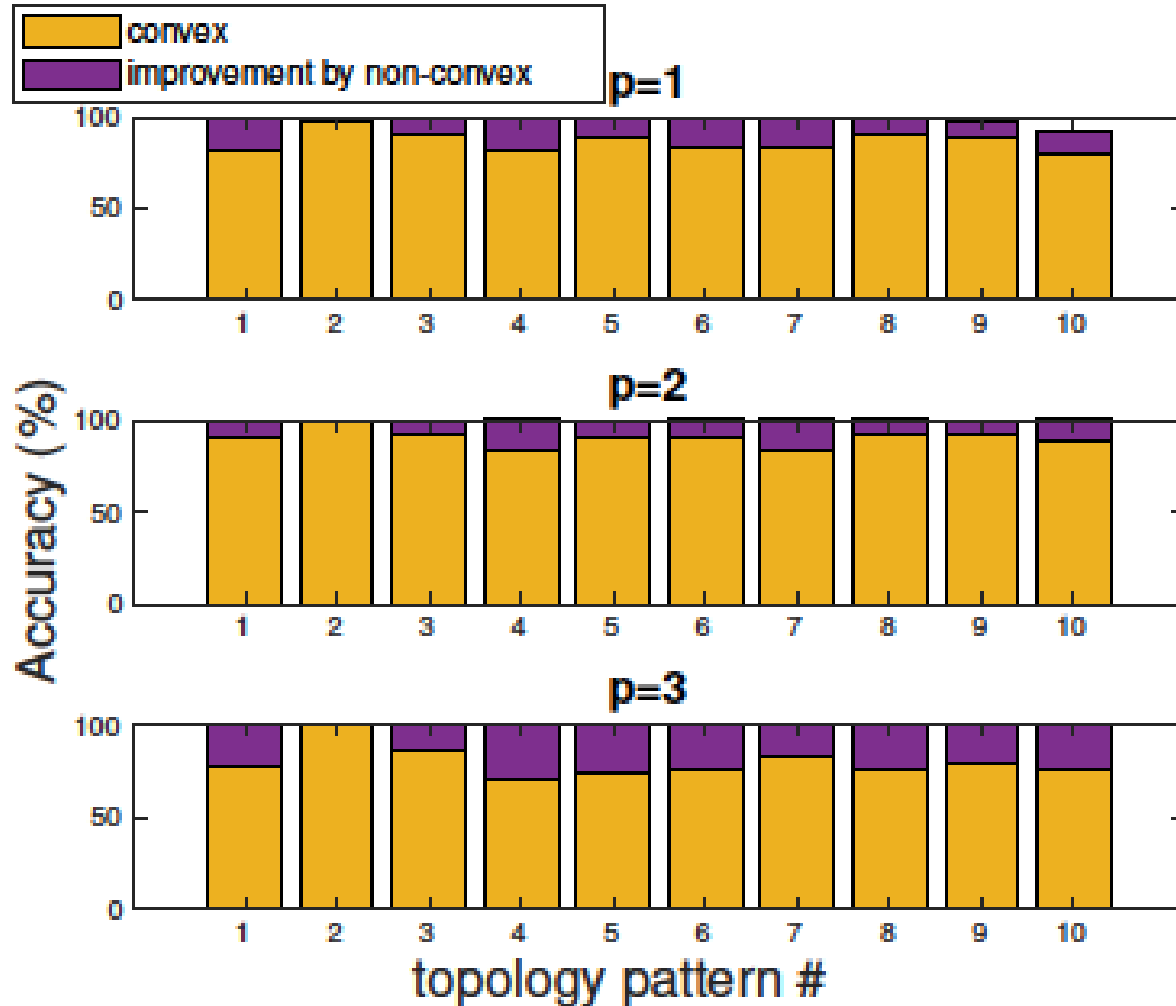
Setting

- 10 GC networks defined on 2nd order 15-dimensional VAR models
- The GC matrix of classifying time-series has sparsity pattern same as one of classes
- Common network density is set to 20%
- vary VAR lag order to test the performance when model order is wrongly chosen

PRELIMINARY RESULTS

Experiment 5: Supervised-classification using learned common Granger network

Result



- Near perfect classification rate in non-convex case
- Non-convex case did not deteriorate much when model order is wrong compared to convex case.

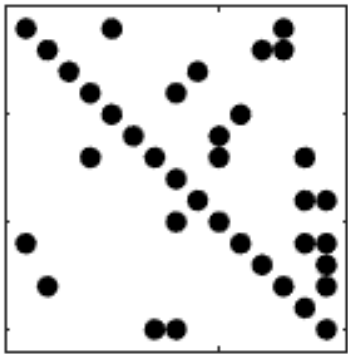
PRELIMINARY RESULTS

Experiment 6: Performance of differential priors

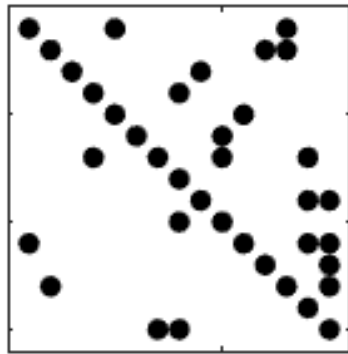
Objective: To illustrate the performance of formulation D

Setting

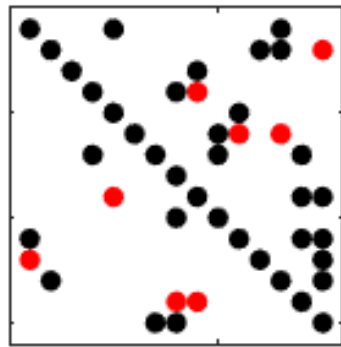
- 4 sets of 15-dimensional 2nd-order-VAR models
- Common network density is set to 20%
- Differential network density is set to 5%
- The ground-truth types are **common type**, **differential type**, **similar type**



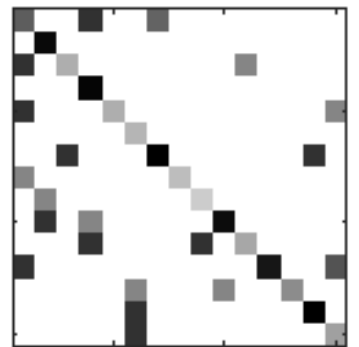
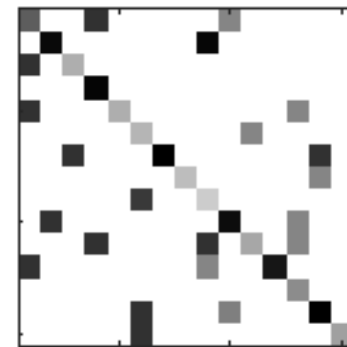
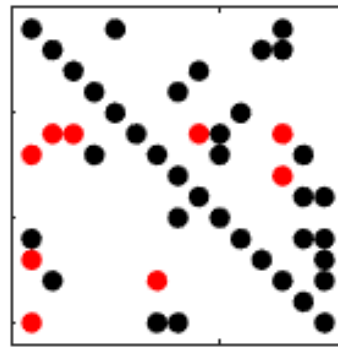
common type



differential type



similar type



PRELIMINARY RESULTS

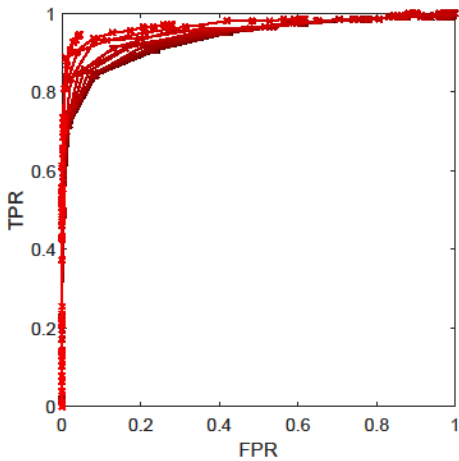
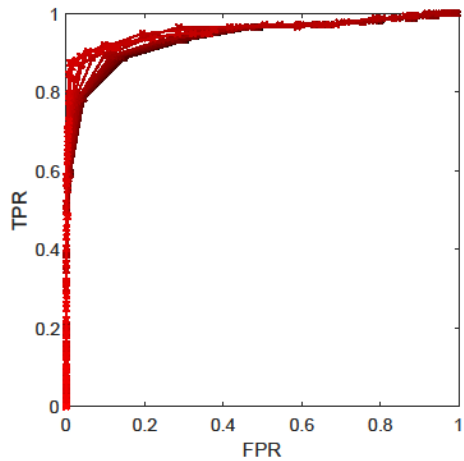
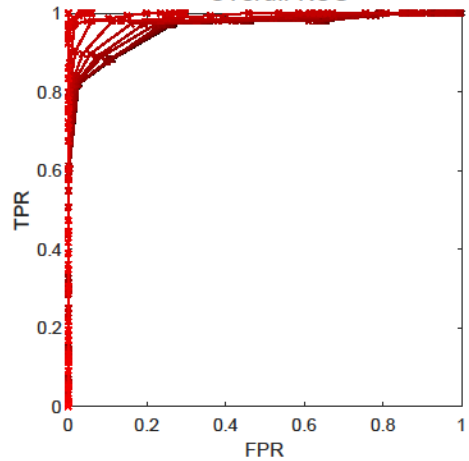
Experiment 6: Performance of differential priors

Ground truth type
D

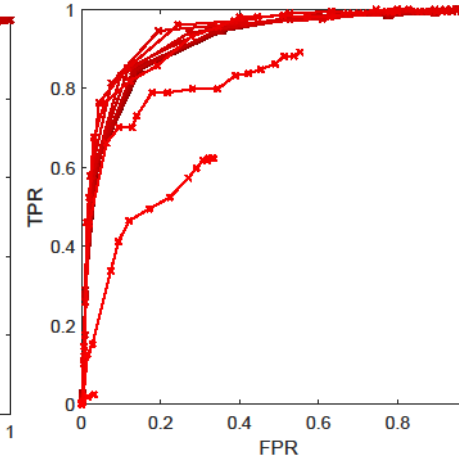
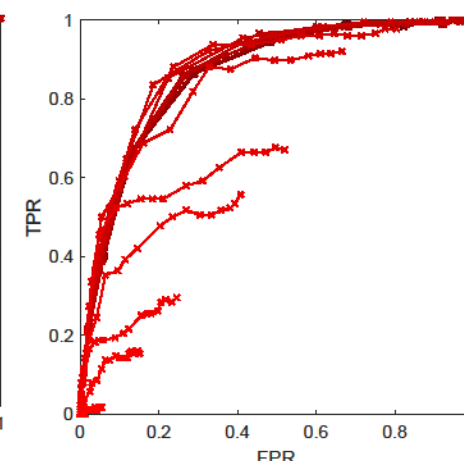
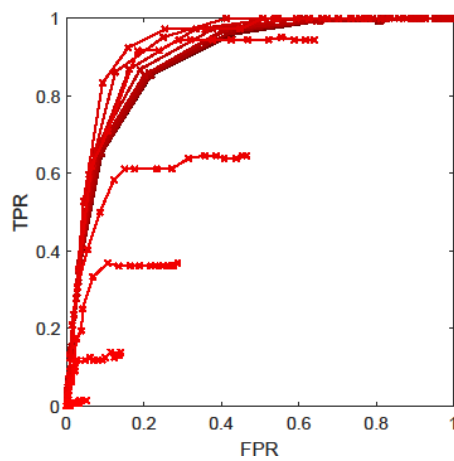
C

D

S



non-convex formulation D
using
Group norm penalty



convex formulation D
using
Group lasso

Overall ROC

FUTURE WORK

Experiments

- Effectiveness of formulations
 - Experiment 4: Common Granger network extraction
 - Experiment 5: Classification
 - Experiment 6: Effectiveness of formulation D
 - Experiment 7: Effectiveness of formulation S
- Brain network application
 - Experiment 8: Application on fMRI time-series

Thesis writing & Publication

"Learning A Common Granger Causality Network Using A Non-Convex Regularization", ICASSP-2020

Formulation C (non-convex)

Goal

- Control the convergence of ADMM algorithm to solve formulation D, S
- Increase performance of algorithms
- Apply formulations on fMRI data

Q&A

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SUPPLEMENTARY: FORMULATION COST FUNCTION

$$(1/2) \|Y^{(k)} - A^{(k)}H^{(k)}\|_2^2$$

Least square (individual)

$$A^{(k)} = [\hat{A}_1^{(k)} \dots, \hat{A}_p^{(k)}]$$

$$B_{ij}^{(k)} = [(A_1^{(k)})_{ij} \dots (A_p^{(k)})_{ij}]$$

$$\sum_{k=1}^K (1/2) \|Y^{(k)} - A^{(k)}H^{(k)}\|_2^2$$

Least square (joint)

$$C_{ij} = [B_{ij}^{(1)} \dots B_{ij}^{(K)}]$$

$$\sum_{k=1}^K \sum_{i \neq j} \|B_{ij}^{(k)}\|_2$$

$$\sum_{k=1}^K \sum_{i \neq j} \|B_{ij}^{(k)}\|_2$$

Regularization

$$\sum_{k=1}^K \sum_{i \neq j} \|C_{ij}\|_2$$

$$\sum_{k=1}^K \sum_{i \neq j} \|C_{ij}\|_2$$

$$\sum_{k < k'} \sum_{i \neq j} \|B_{ij}^k - B_{ij}^{k'}\|_2$$

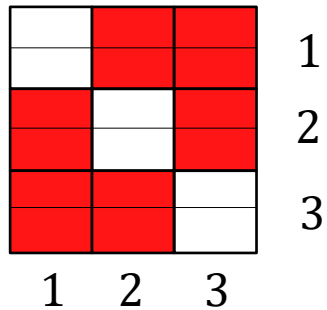
Formulation C

Formulation D

Formulation S

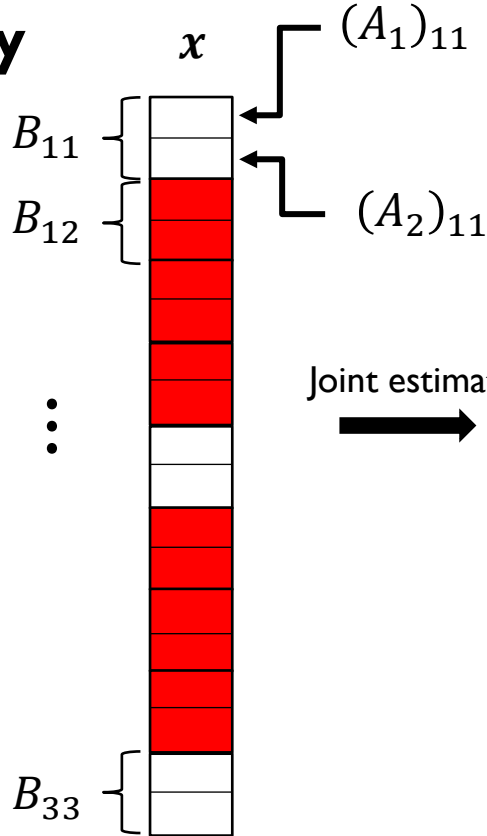
SUPPLEMENTARY

Group norm penalty



1
2
3

vectorize
→



Stacked VAR coefficient matrix

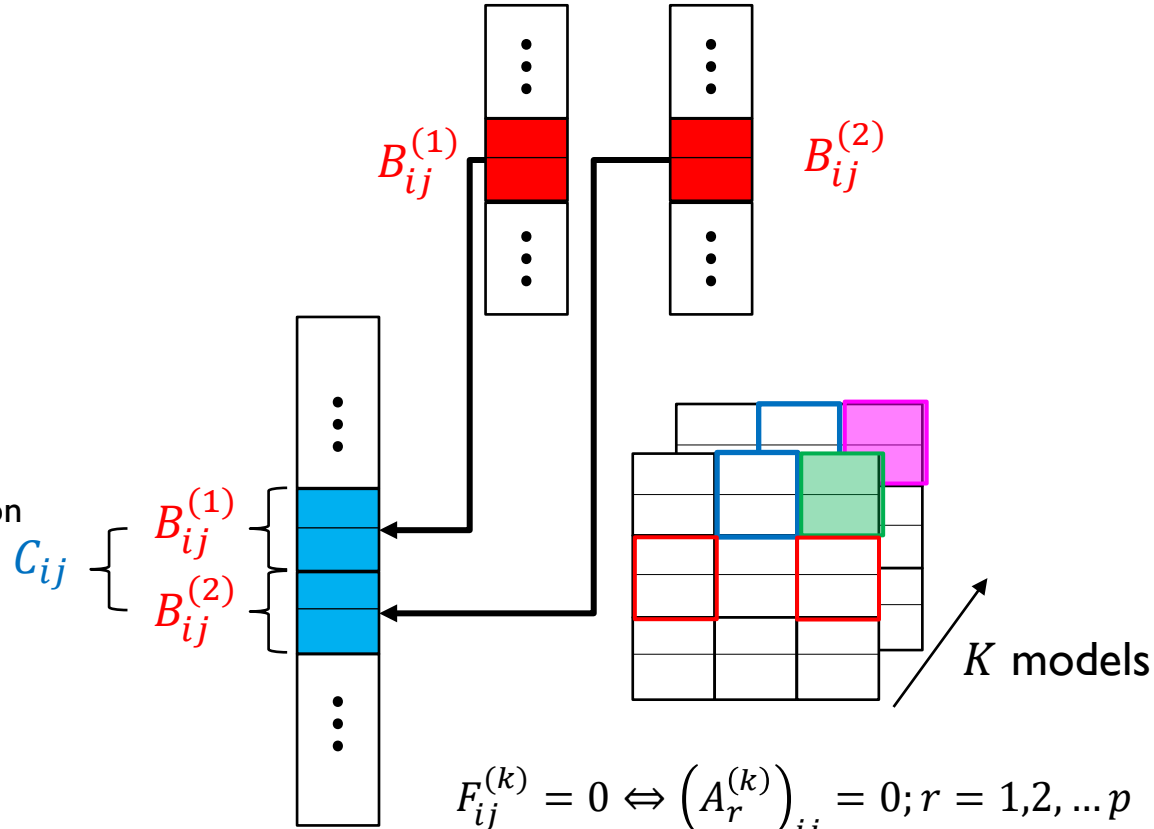
Knowing that the sparsity must be a block of size p

↓

Penalize $\sum_{i \neq j} \|B_{ij}\|_2^q \rightarrow \boxed{\|Px\|_{2,q}^{(p)}}$

$q = 1$, Group lasso
 $q = 1/2$, **Our non-convex extension**

Joint estimation
→



$$F_{ij}^{(k)} = 0 \Leftrightarrow (A_r^{(k)})_{ij} = 0; r = 1, 2, \dots, p$$

- Penalize $\sum_{i \neq j} \|C_{ij}\|_2^q \rightarrow \boxed{\|Px\|_{2,q}^{(pK)}}$
- Penalize $\sum_{m \neq l} \sum_{i \neq j} \|B_{ij}^{(m)} - B_{ij}^{(l)}\|_2^q \rightarrow \boxed{\|Dx\|_{2,q}^{(p)}}$
- Penalize $\sum_k \sum_{i \neq j} \|B_{ij}^{(k)}\|_2^q \rightarrow \boxed{\|Px\|_{2,q}^{(p)}}$

$$\text{C. } \min_x \|y - Gx\|_2^2 + \lambda \|Px\|_{2,q}^{(pK)}$$

$$\text{D. } \min_x \|y - Gx\|_2^2 + \lambda_1 \|Px\|_{2,q}^{(p)} + \lambda_2 \|Px\|_{2,q}^{(pK)}$$

$$\text{S. } \min_x \|y - Gx\|_2^2 + \underbrace{\lambda_1 \|Px\|_{2,q}^{(p)} + \lambda_2 \|Dx\|_{2,q}^{(p)}}_{\substack{g(z) \\ \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} x - z = 0}}$$

SUPPLEMENTARY : ADMM STEP

$$x^+ = \operatorname{argmin}_x \|Gx - b\|_2^2 + \frac{\rho}{2} \left\| \begin{bmatrix} L_1 \\ L_2 \end{bmatrix} x - z + \frac{y}{\rho} \right\|_2^2$$

$$z^+ = \min_{z_1, z_2} \lambda_1 \|z_1\|_{2,q}^{(M_1)} + \lambda_2 \|z_2\|_{2,q}^{(M_2)} + \frac{\rho}{2} \left\| \begin{bmatrix} L_1 \\ L_2 \end{bmatrix} x - z + \frac{y}{\rho} \right\|_2^2$$

$$y^+ = y + \rho \begin{bmatrix} L_1 \\ L_2 \end{bmatrix} x - z$$

Monotone accelerated proximal gradient (mAPG)

Beck & Teboulle

Descent

$$y_k = x_k + \frac{t_{k-1} - 1}{t_k} (x_k - x_{k-1}) + \frac{t_{k-1}}{t_k} (z_k - x_k)$$

$$t_{k+1} = 0.5(1 + \sqrt{1 + 4t_k^2})$$

$$z_{k+1} = \text{prox}_{\lambda g}(y_k - \lambda \nabla f(y_k))$$

$$x_{k+1} = \text{argmin}\{F(x_k), F(z_{k+1})\} \text{ Monitoring step}$$



Does not generate sufficient decreasing sequence.

Monotone accelerated proximal gradient (mAPG)

Beck & Teboulle 

Li & Lin

Descent 

Sufficient descent

$$y_k = x_k + \frac{t_{k-1} - 1}{t_k} (x_k - x_{k-1}) + \frac{t_{k-1}}{t_k} (z_k - x_k)$$

$$t_{k+1} = 0.5(1 + \sqrt{1 + 4t_k^2})$$

$$z_{k+1} = \text{prox}_{\lambda g}(y_k - \lambda \nabla f(y_k)) \quad \text{Compute original proximal gradient step} \quad \Rightarrow \quad v_{k+1} = \text{prox}_{\lambda g}(x_k - \lambda \nabla f(x_k))$$

$$x_{k+1} = \text{argmin}\{F(v_{k+1}), F(z_{k+1})\} \quad \text{Monitoring step} \quad \Rightarrow \quad \text{Sufficient descent}$$


Monotone APG is proved to converge in some **non-convex** problems.

However, monitoring step is **too conservative**.

Monotone accelerated proximal gradient (mAPG)

Beck & Teboulle 

Li & Lin

Descent 

Sufficient descent

$$y_k = x_k + \frac{t_{k-1} - 1}{t_k} (x_k - x_{k-1}) + \frac{t_{k-1}}{t_k} (z_k - x_k)$$

$$t_{k+1} = 0.5(1 + \sqrt{1 + 4t_k^2})$$

$$z_{k+1} = \text{prox}_{\lambda g}(y_k - \lambda \nabla f(y_k))$$

$$F(z_{k+1}) \leq F(x_k) - \delta \|z_{k+1} - x_k\|_2^2?$$

YES

NO

$x_{k+1} = z_{k+1}$
No proximal step

$x_{k+1} = \text{prox}_{\lambda g}(x_k - \lambda \nabla f(x_k))$

Can **sufficient descent property** can be dropped in non-convex setting ?

There is a **trick**.

SUPPLEMENTARY

Non-monotone accelerated proximal gradient (nmAPG)

In objective function

Beck & Teboulle



Li & Lin

Descent



Sufficient descent

$$y_k = x_k + \frac{t_{k-1} - 1}{t_k} (x_k - x_{k-1}) + \frac{t_{k-1}}{t_k} (z_k - x_k)$$

$$t_{k+1} = 0.5(1 + \sqrt{1 + 4t_k^2})$$

$$z_{k+1} = \text{prox}_{\lambda g}(y_k - \lambda \nabla f(y_k))$$

$$F(z_{k+1}) \leq c_k - \delta \|z_{k+1} - y_k\|_2^2?$$

YES

NO

$x_{k+1} = z_{k+1}$
No proximal step

Monitoring step in mAPG

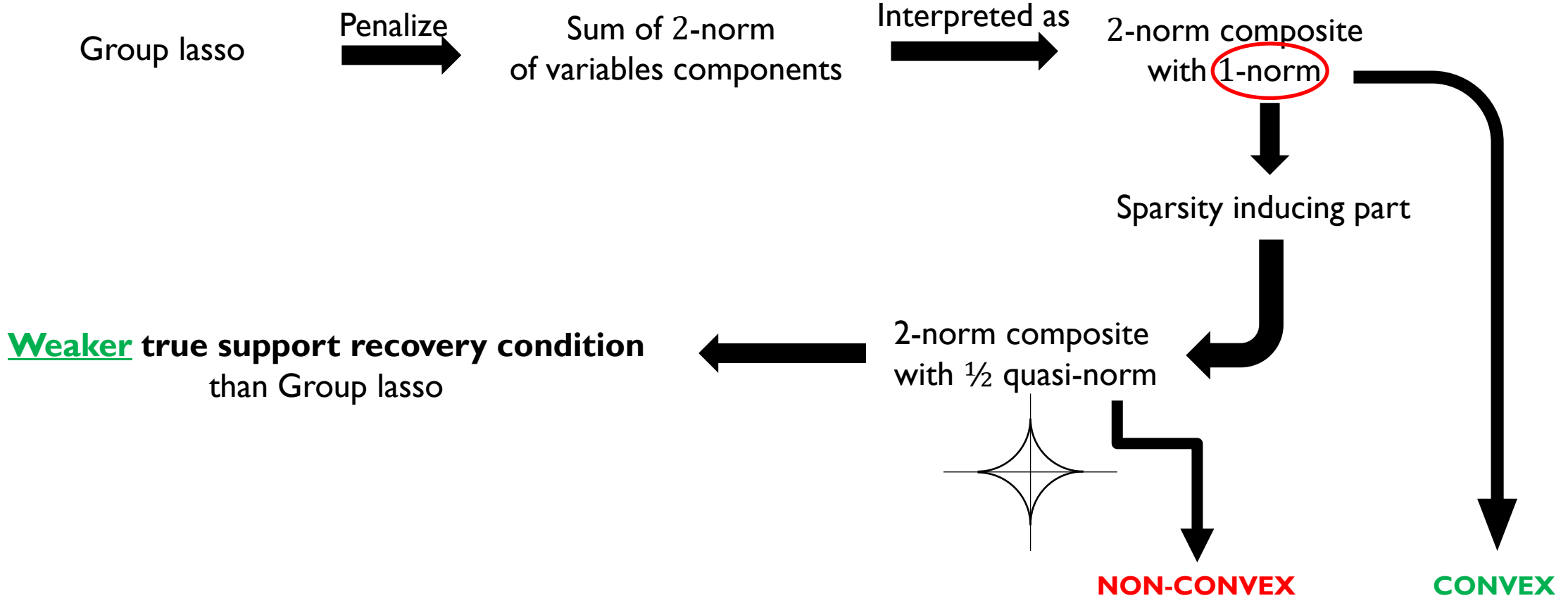
$$x_{k+1} = \text{argmin}\{F(v_{k+1}), F(z_{k+1})\}$$

c_k is weighted average of objective function in iterations $1, \dots, k$.

Sequence c_k is strictly monotone decreasing while $F(x_k)$ may not.

SUPPLEMENTARY

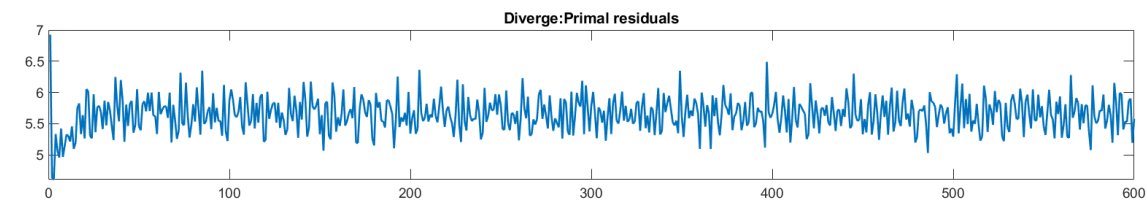
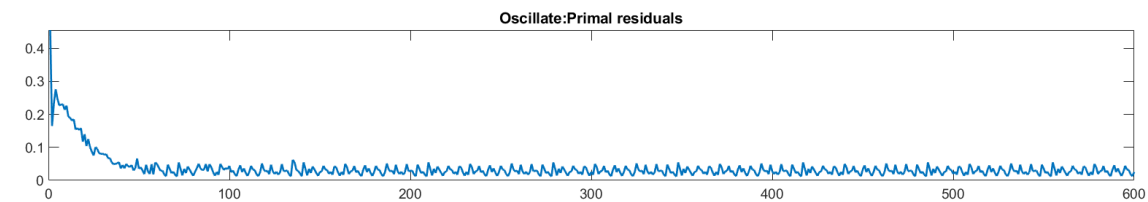
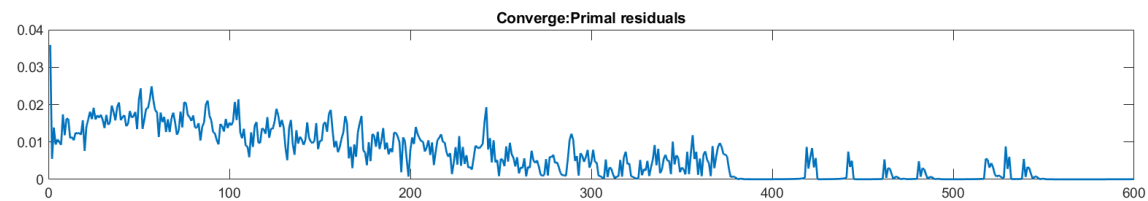
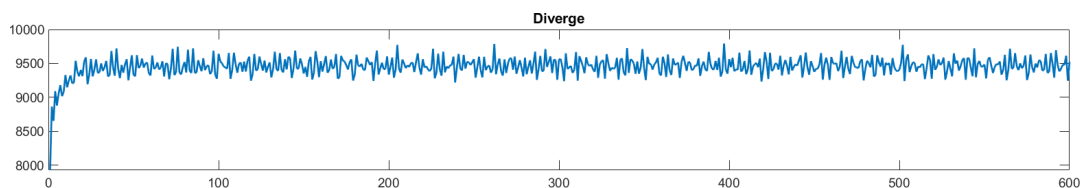
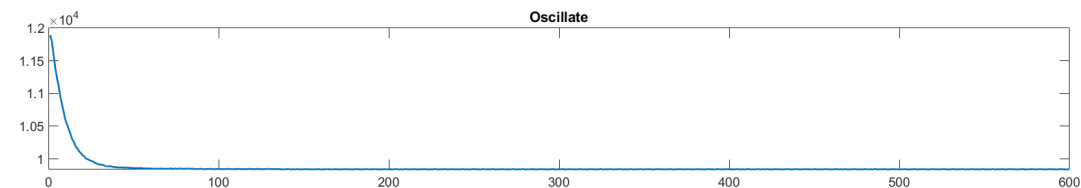
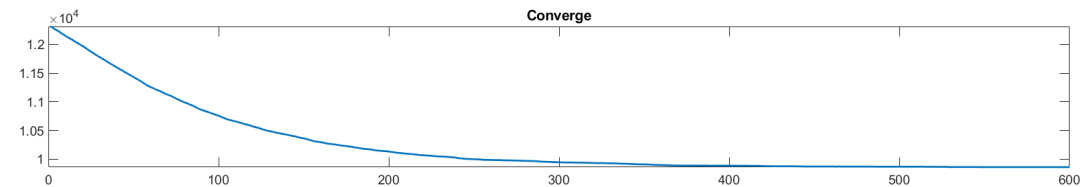
Choices of sparsity inducing-penalty



SUPPLEMENTARY

ADMM convergence issues

$$\min_{Ax+Bz=c} f(x) + g(z)$$



$$f(x) + g(z)$$

$$\|Ax + Bz - c\|_2$$

$$\mathcal{L}(x, z, y, \rho) = f(x) + g(z) + y^T r + \frac{\rho}{2} \|r\|_2^2$$

$$r = (Ax + Bz - c)$$