# Joint Gaussian Graphical Model Series – VIII A deep introduction of the metrics for evaluating an/a estimator/learner

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Sep 22nd, 2017

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# Road Map



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# Outline





- 3 The metrics for evaluating an estimator
- 4 Statistical Convergence Rate
- 5 Optimization Convergence Rate
- 6 Computational Complexity

# Notation

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## Notation

- X The data matrix
- $\Sigma$  The covariance matrix.
- $\Omega$  The precision matrix.
- *p* The number of features.
- *n* The number of samples in the data matrix.
- s The number of non-zero entries in the precision matrix.

# Review

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• We introduce different sGGM estimators and their solution.

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- We introduce different sGGM estimators and their solution.
- We briefly introduce the three metrics used in evaluating an estimator.

- We introduce different sGGM estimators and their solution.
- We briefly introduce the three metrics used in evaluating an estimator.
- We introduce different multi-task sGGMs estimators and their optimization challenges.

#### The metrics for evaluating an estimator

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#### Motivation I: Select a proper estimator

• There may be a lot of similar estimators.



#### Motivation I: Select a proper estimator

- There may be a lot of similar estimators.
- You need to decide which one to use.



#### Motivation I: Select a proper estimator

- There may be a lot of similar estimators.
- You need to decide which one to use.
- You need some metrics to make the decision.



#### Motivation II: Evaluate a novel method

• You may come out a new estimator.

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- You may come out a new estimator.
- You want to know whether this novel estimator is no worse than the previous ones.

- You may come out a new estimator.
- You want to know whether this novel estimator is no worse than the previous ones.
- Then you need some metrics to evaluate the estimator.

10 / 30

# Background: Two major properties

• Two major properties: Accuracy and Speed.

Image: A match a ma

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# Background: Two major properties

- Two major properties: Accuracy and Speed.
- Accuracy:
  - Statistical Convergence rate
  - how close to the Truth
  - Statisticians

# Background: Two major properties

- Two major properties: Accuracy and Speed.
- Accuracy:
  - Statistical Convergence rate
  - how close to the Truth
  - Statisticians
- Speed:
  - Optimization convergence rate
  - Optimization researchers
  - Computational complexity
  - Computer Scientists



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#### Statistical Convergence Rate

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13 / 30

#### Statistical Convergence Rate : Definition

• The task for an estimator is parameter estimation.

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#### Statistical Convergence Rate : Definition

- The task for an estimator is parameter estimation.
- Suppose the parameter you need to estimate is  $\theta,$  the truth is  $\theta^*$

- The task for an estimator is parameter estimation.
- Suppose the parameter you need to estimate is  $\theta$ , the truth is  $\theta^*$

• 
$$\| \theta - \theta^* \|$$
 or  $\mathcal{R}(\theta - \theta^*)$ 

#### A simple example: Estimate the mean

On the whiteboard.

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15 / 30

Elementary Estimator[Yang et al.(2014b)Yang, Lozano, and Ravikumar]

$$\underset{\theta}{\operatorname{argmin}} \mathcal{R}(\theta) \tag{4.1}$$
Subject to:  $\mathcal{R}^*(\theta - \mathcal{B}^*(\widehat{\phi})) \leq \lambda_n$ 
(4.2)

Here  $\mathcal{B}^*(\phi)$  is a backward mapping for  $\phi$ .

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Example: sparse linear regression[Yang et al.(2014a)Yang, Lozano, and Ravikumar]

$$\underset{\theta}{\operatorname{argmin}} ||\theta||_{1}$$
Subject to:  $||\theta - (X^{T}X + \epsilon I)^{-1}X^{T}y||_{\infty} \le \lambda_{n}$ 
(4.3)

17 / 30

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# Hands on: Elementary Estimator for high-dimensional linear regression

On the whiteboard.

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18 / 30

# Hands on: DIFFEE

On the whiteboard.

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- In high-dimensional setting, related to  $\frac{\log p}{n}$ .
- Equivalent estimators still have differences in constants or constraints

#### **Optimization Convergence Rate**

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• Linearly Converge: 
$$\lim_{k \to \infty} \frac{|\theta_{k+1} - L|}{|\theta_k - L|} = \mu_k$$

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- Linearly Converge:  $\lim_{k \to \infty} \frac{|\theta_{k+1} L|}{|\theta_k L|} = \mu_k$
- Linearly, if  $\mu_k \in (0,1)$ 
  - Superlinearly, if  $\mu_k \to 0$  when  $k \to \infty$ .
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• Higher order: 
$$\lim_{k \to \infty} \frac{|x_{k+1}-L|}{|x_k-L|^q} > 0.$$

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- Closed form solution
- Closed form  $\geq$  Higher order  $\geq$  linear

• Gradient Descent based method: Linear

Image: A math a math

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- Gradient Descent based method: Linear
- Figure gradient descent
  - SGD
  - ADMM / proximal gradient descent

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- Gradient Descent based method: Linear
- Figure gradient descent
  - SGD
  - ADMM / proximal gradient descent
- Newton method based method: Quadratic
- Elementary Estimator: Closed form solution

# Optimization Convergence Rate: Different methods

	Single s	GGM	Multiple sGGMs		
Method:	GLasso	CLIME	EEGM	JGL	FASJEM
Rate of Convergence	Linear	NA	Closed form	Linear	Linear

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#### Computational Complexity

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# Computational Complexity: Definition

• Complexity of an algorithm is the amount of resources required for running it.

26 / 30

# Computational Complexity: Definition

- Complexity of an algorithm is the amount of resources required for running it.
- In machine learning, it is mainly related to *n* and *p*.

# Computational Complexity: Definition

- Complexity of an algorithm is the amount of resources required for running it.
- In machine learning, it is mainly related to *n* and *p*.
- Use big O notation

# Computational Complexity: how to calculate

#### • Some cases:

- Matrix Multiplication: O(np<sup>2</sup>)
- Matrix inversion O(p<sup>3</sup>)
- SVD inversion O(p<sup>3</sup>)
- ▶ soft-thresholding O(p<sup>2</sup>)

# Computational Complexity: how to calculate

#### • Some cases:

- Matrix Multiplication: O(np<sup>2</sup>)
- Matrix inversion O(p<sup>3</sup>)
- SVD inversion O(p<sup>3</sup>)
- soft-thresholding O(p<sup>2</sup>)
- How to calculate:
  - Num of Iter × Computational complexity of each Iter
  - Direct calculate e.g., Closed form solution
  - Use existing method e.g., linear programming
  - Special case: linear convergence.

# Computational Complexity: Different methods

	Single sGGM			Multiple sGGMs		
Method:	GLasso	CLIME	EEGM	JGL	FASJEM	SIMUL
Computational Complexity	<i>O</i> ( <i>Tp</i> <sup>2</sup> )	$O(p^5)$	$O(p^2)$	<i>O</i> ( <i>Tp</i> <sup>3</sup> )	$O(Tp^2)$	<i>О</i> (К <sup>4</sup> р

Beilun Wang, Advisor: Yanjun Qi (University Joint Gaussian Graphical Model Series – VIII

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- We introduce the statistical convergence rate.
- We introduce the optimization convergence rate.
- We introduce the computational complexity.

29 / 30

#### References I

 E. Yang, A. Lozano, and P. Ravikumar.
 Elementary estimators for high-dimensional linear regression.
 In Proceedings of the 31st International Conference on Machine Learning (ICML-14), pages 388–396, 2014a.

 E. Yang, A. C. Lozano, and P. K. Ravikumar. Elementary estimators for graphical models.
 In Advances in Neural Information Processing Systems, pages 2159–2167, 2014b.