

Disc-GLasso: Discriminative Graph Learning with Sparsity Regularization

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Motivation

Graph structures are natural to use

- Construct optimal graph not trivial
 - benefit subsequent data analysis & could learn from data
- Prior art learn graphs w.r.t.
 - Representability: benefits energy compaction
 - Sparsity: benefits interpretation

Objectives

- Multi-class classification among data samples (graph signals)
- Develop approach to learn a set of graphs that benefits classification

Key Contributions

- First propose multi-graph learning that promotes discrimination
- Develop efficient algorithm to learn discriminative class-specific graphs

Problem Formulation

Notations

- random graph signals in i -th class: $\mathbf{x}^{(i)} \in \mathbb{R}^n$
- S classes in total
- For i -th class, N_i i.i.d. realizations/samples: $\mathbf{x}_1^{(i)}, \dots, \mathbf{x}_{N_i}^{(i)}$
- \mathbf{K}_i : empirical cov. matrix of samples in i -th class

Define **multi-category graph learning** problem:

Goal: learn graph structure of each category, $\mathcal{G}_1, \dots, \mathcal{G}_S$

- $\mathcal{G}_i = (\mathcal{V}, \mathcal{E}_i, \mathbf{Q}_i)$, n-vertex set \mathcal{V} , edge set \mathcal{E}_i
- Symmetric matrix representation \mathbf{Q}_i , where $\forall a \neq b, (a, b) \in \mathcal{E}_i \iff \mathbf{Q}_{i,ab} \neq 0$
- \mathbf{Q}_i is only required to be positive semi-definite

Baseline Approach

Apply graphical lasso indep. to each class:

- Solve ℓ_1 -penalized Gaussian ML estimation problem separately for the graph of each category i ,

$$\begin{aligned} \min -\log \det(\mathbf{Q}_i) + \text{tr}(\mathbf{K}_i \mathbf{Q}_i) + \rho \|\mathbf{Q}_i\|_1 \\ - \text{tr}(\mathbf{K}_i \mathbf{Q}_i) = \frac{1}{N_i} \sum_{k=1}^{N_i} \mathbf{x}_k^{(i)T} \mathbf{Q}_i \mathbf{x}_k^{(i)} \\ - \text{Minimize above term} \Rightarrow \text{promote smoothness of data samples in } i\text{-th class on } i\text{-th graph} \end{aligned}$$

- Only favor energy compaction and sparsity within each class
- Discrimination between classes not guaranteed

Disc-GLasso Algorithm

For each \mathbf{W}_i , given the empirical covariance matrices $\mathbf{K}_1, \dots, \mathbf{K}_S$.

1. Search for the minimum ratio r such that $\mathbf{K}_i - \frac{1}{r} \sum_{j \neq i}^S \mathbf{K}_j \succeq 0, \forall i$.
2. Initialize with $\mathbf{W}_i = \mathbf{K}_i + \rho \mathbf{I} - \frac{1}{r} \sum_{j \neq i}^S \mathbf{K}_j$. The diagonal of \mathbf{W}_i will remain unchanged in what follows.
3. Perform following steps until convergence reached:
 - (a) Rearrange the rows/columns so that the target column is last.
 - (b) Solve the lasso problem for $\hat{\beta}$:

$$\arg \min_{\beta} \frac{1}{2} \left\| \mathbf{W}_{11}^{i-1/2} \beta - \mathbf{W}_{11}^{i-1/2} \mathbf{k}_{12}^i + \frac{1}{r} \sum_{j \neq i}^S \mathbf{W}_{11}^{i-1/2} \mathbf{k}_{12}^j \right\|^2 + \rho \|\beta\|_1$$

- (c) Fill in the corresponding row and column of \mathbf{W}_i using $\mathbf{w}_{12}^i = \mathbf{W}_{11}^{i-1/2} \hat{\beta}$.

Proposed Solution

- Key idea: jointly learn the graphs for all classes by promoting
 - Smoothness of data in i -th class on i -th graph
 - Non-smoothness on learned graphs corresponding to the other classes
- To achieve above properties, we need to minimize the following,

$$\sum_{i=1}^S \sum_{k=1}^{N_i} \frac{1}{N_i} \left[\mathbf{x}_k^{(i)T} \mathbf{Q}_i \mathbf{x}_k^{(i)} - \frac{1}{S-1} \sum_{j \neq i}^S \mathbf{x}_k^{(i)T} \mathbf{Q}_j \mathbf{x}_k^{(i)} \right]$$
- Finally, we propose to solve the optimization problem below.

$$\min_{\mathbf{Q}_i \succeq 0} -\log \det(\mathbf{Q}_i) + \text{tr}(\mathbf{K}_i \mathbf{Q}_i) - \frac{\mu_i}{S-1} \sum_{j \neq i}^S \text{tr}(\mathbf{K}_j \mathbf{Q}_i) + \rho_i \|\mathbf{Q}_i\|_1, \quad (1)$$
 for each \mathbf{Q}_i , given $\mathbf{K}_1, \dots, \mathbf{K}_S$.
- A block coordinate descent based algorithm is developed to solve (1).

Parameter Choice: Let $r = \frac{S-1}{\mu}$,

- Smaller $r \Rightarrow$ better discrimination
- Need to ensure $\mathbf{K}_i - \frac{1}{r} \sum_{j \neq i}^S \mathbf{K}_j \succeq 0, \forall i$ to guarantee that after each updating step t , $\mathbf{W}_i^{(t)} \succ 0, \forall t$.

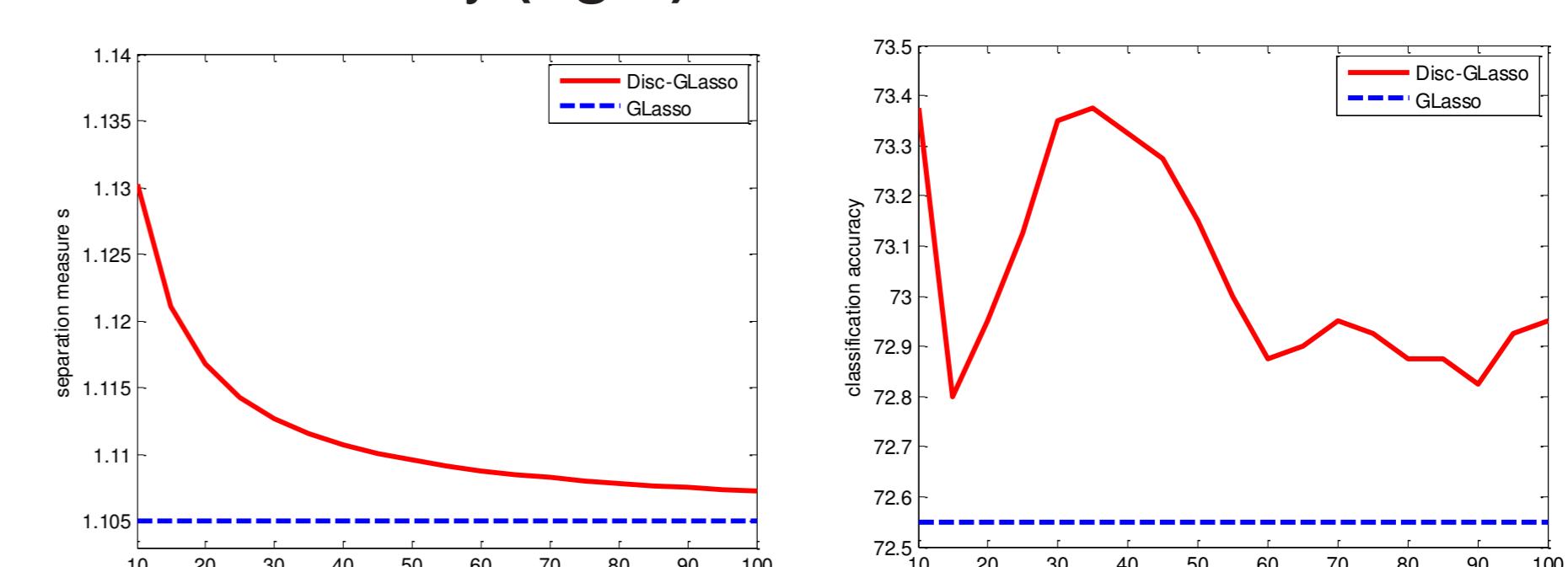
In proposed algorithm, we search for the minimum r s.t. $\mathbf{K}_i - \frac{1}{r} \sum_{j \neq i}^S \mathbf{K}_j \succeq 0, \forall i$, via line search through predefined set of values.

- the only additional time cost of our algorithm compared to GLasso

Experiments

Synthetic data for binary classification

- From left to right: $\mathcal{G}_1, \mathcal{G}_2$ learned with GLasso, and $\mathcal{G}_1, \mathcal{G}_2$ learned with Disc-GLasso.
- Cumulative spectrum energy of test signals in class 1 (left) and class 2 (right) on the learned graphs.
- Effect of r on the separation measure $s = \frac{\text{tr}(\mathbf{K}_1 \mathbf{Q}_2) + \text{tr}(\mathbf{K}_2 \mathbf{Q}_1)}{\text{tr}(\mathbf{K}_1 \mathbf{Q}_1) + \text{tr}(\mathbf{K}_2 \mathbf{Q}_2)}$ (left) and classification accuracy (right).



References

1. J. Friedman et.al, "Sparse inverse covariance estimation with the graphical lasso," Biostatistics, 2008.
2. R. Mazumder and T. Hastie, "The graphical lasso: New insights and alternatives," Elect. journal of stat., 2012.