Node wise Lasso - LIN

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2.2 Simulation

For the target of comparing the sample performance (such as False Positives, False Negatives) between Node-wise Lasso approach and Graphical Lasso approach, simulation data is generated by the following settings:

Consider the p-dimensional multivariate Gaussian distributed random variable

$$\boldsymbol{X} = (X_1, X_2, ..., X_p)^T \sim \mathcal{N}(0, \boldsymbol{\Sigma})$$

, where $\boldsymbol{\Sigma} = \boldsymbol{\Theta}^{-1}$.

In detail, we let $\boldsymbol{\Theta} = \boldsymbol{B} + \delta \boldsymbol{I_p} \in \mathbb{R}^{p \times p}$ where $\boldsymbol{I}_p$ stands for the identity matrix and symmetric matrix $\boldsymbol{B}$ has its each off-diagonal entry generated respectively and independently, which will equal to 0 with probability 0.9 or equal to 0.5 with probability 0.1. We calculated and chose $\delta > 0$ to guarantee $\boldsymbol{\Theta}$ is positive definite. We standardized the $\boldsymbol{\Theta}$ to achieve correlation matrix instead of covariance matrix.

Of particular interest is the identification of entries that equals to 0 in the $\boldsymbol{\Theta}$, the sparsity pattern in $\boldsymbol{\Theta}$ links to the true edge set E in the graphical model $G = (V, E)$, where $V = 1, ..., p$ is the set of nodes and E is the set of edges $\in V \times V$ between nodes.

Finally, we can specify two arguments in the `simulation(n, p)` function, with `n` as the number of dataset generated, and with `p` as the number of dimension or, say, the number of nodes generated in $\boldsymbol{X} = (X_1, X_2, ..., X_p)^T$. As the return of the function, a list consisting of:

1. A $n \times p$ data set.
2. $\boldsymbol{\Theta}$
3. Standardized $\boldsymbol{\Theta}$

For instance, an 100×50 dataset is generated by the following codes.

```
data_list <- simulation(50,100)
simulation_data <- data_list$data
simulation_StandardTheta <- data_list$standardtheta
```

To have a stable and reliable result, we are conducting 50 iterations and having mean value of the results from all the method introduced and discussed in the following chapters. ## 2.3 Node-wise Lasso approach

2.3.1 Introduction

One of the approaches that has been deployed to estimate the edge set E is based on the linear regression. Under the assumption of $\boldsymbol{X}$ being multivariate Gaussian distributed random variable, the method of node-wise Lasso is estimate each random variables X_i in $\boldsymbol{X} = (X_1, X_2, ..., X_p)^T$ by applying linear regression on the remaining variables. More specifically, for each node $i \in V$, we regress X_j on the remaining variables $X_j = \{X_j : j \in V, j \neq i\}$ to achieve this form

$$X_i = \sum_{1 \leq j \leq p, j \neq i} \beta_{ij} X_j + \epsilon_{ij}$$

Due to the high dimensionality of our setting, we could implement the Lasso method while regressing all variables to achieve sparse solution.

For response variable y_i and predicators x_{ij}, the lasso coefficient $\hat{\beta_\lambda}$ is chosen to minimise the equation

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}|\beta_j|$$

where $\lambda \geq 0$ is the tuning parameter. As the l_1 norm of penalty has the effect of forcing some fo the coefficients to be exactly zero where a large enough λ is chosen, Lasso can perform variable selection and build a sparse model containing a subset of all p predictors.

Section 2.3.3 will introduce and compare different method to choose optimal tuning parameter λ and the performance each of them achieves. After choosing the tuning parameter λ, we could attain the Lasso estimation for each coefficient β_{ij}, which is $\hat{\beta_{ij}}$. we consider the following rules, named **node-wise Lasso 1** and **node-wise Lasso 2** to estimate the Edge Set E:

1. **node-wise Lasso 1**: if $\hat{\beta_{ij}} \neq 0$ and $\hat{\beta_{ji}} \neq 0$ are satisfied, then we say nodes X_i and X_j are estimated to be connected.
$$\hat{E_1}=\left\{(i,j):\hat{\beta_{ij}},\hat{\beta_{ji}}\neq 0, 1\leq i,j\leq p, i\neq j\right\}$$
2. **node-wise Lasso 2**: if either $\hat{\beta_{ij}}=0$ or $\hat{\beta_{ji}}=0$, we say nodes X_i and X_j are estimated to be connected.
$$\hat{E_2}=\left\{(i,j):\exists\hat{\beta_{ij}},\hat{\beta_{ji}}\neq 0, 1\leq i,j\leq p, i\neq j\right\}$$

For each rule and a certain choice of the tuning parameter λ, by comparing the true edge set E and the estimated edge set $\hat{E}$, the elements in the Confusion Matrix can be calculated and based on that, the True Positive Rate (TPR_λ) and False Postive Rate (FPR_λ) can be attained consequently. As a result, we are able to plot the ROC curve over a fine grid of values of λ. Furthermore, the Area Under the ROC ($AUROC$) for each method will be plotted to compare the overall performance on recovering the true edge set E. These will be introduced in the ***Chapter 2.3.2***.

2.3.2 ROC Curve

After conducting node-wise lasso with different tuning parameter λ and different choices of method ($\hat{E_1}$ and $\hat{E_2}$), one way to compare their performance is to plot the Receiver Operating Characteristic Curve (ROC Curve), created by plotting the true positive rate (TPR_λ) against the false positive rate (FPR_λ) at various choices of λ. ROC analysis provides us methods to select potentially optimal models and to compare the performance. Further interpretations such as Area Under Curve (AUC) can be calculated for more analysis.

For each specific λ, Lasso estimation for each coefficient β_{ij} can be achieved, here in the function `edge_table(data_set, lambda_choice)`. By treating the simulated data and lambda choice, the function will return a $p \times p$ matrix where each entry will be either `TRUE` or `FALSE` which respectively suggests that, for example, at (i,j)-entry, `TRUE` means $\hat{\beta_{ij}} \neq 0$ and `FALSE` means $\hat{\beta_{ij}}=0$. Corresponds to the rules **node-wise Lasso 1**, we say nodes i and j are estimated to be connected as long as Both (i,j)-entry and (j,i)-entry are `TRUE`. Equivalently, **node-wise Lasso 2** only requires either (i,j)-entry or (j,i)-entry are `TRUE` for connecting nodes i and j.

Since the sparsity pattern in the $\mathbf{\Theta}$ identifies the true edge set E

$$E=\{(i,j):\Theta_{ij}\neq 0, 1\leq i,j\leq p, i\neq j\}$$

, function `true_edge(theta)` visualises these and return a $p \times p$ matrix similar to the one returned by the function `edge_table(data_set, lambda_choice)`.

Finally,by making the results from `edge_table` and `true_edge` as arguments function `confusion_matrix(estimate_edge, trueedge, estimate_way)` will perform calculation of confumatrix and return relevant result including TPR_λ and FPR_λ. Setting `estimate_way = "both"` will allow function perform the calculation through **node-wise Lasso 1**, while `estimate_way = "either"` makes it go through **node-wise Lasso 2**.

As a result, each λ will leads to a specific pair of TPR_λ and FPR_λ, function `ROC_curve` automates this process by computing through all the lambda and return all the coordinates (TPR_λ,FPR_λ).

ROC Curve of different methods with same p and n.

In this section, the ROC Curves of methods $\hat{E_1}$ and $\hat{E_2}$ will be compared in parallel with p and n being controlled. we conducted each of the methods mainly under three circumstances:

1. $n < p$
2. $n = p$
3. $n > p$

First of all, for $p = 20$ and $n = 1000$, which leads to the ratio $\frac{p}{n} = 0.02$, we have the following ROC curve (*Figure 2.3.2.2*). In this low $\frac{p}{n}$ ratio settings, a large enough volumn of training data will help to achieve a good optimal performance on both methods and $\hat{E_2}$ has slightly higher AUC than the $\hat{E_1}$. More specifically, $\hat{E_1}$ has $AUC = 0.99199$ while $AUC = 0.99140$ for $\hat{E_2}$.(Under 50-times iterations setting).

Secondly, for $p = 100$ and $n = 100$, which leads to the ratio $\frac{p}{n} = 1$, we have the following ROC curve (*Figure 2.3.2.3*). In this case, we have a low number of observations and also a relatively high $\frac{p}{n}$ ratio, both methods achieved a lower performance compared to the last case. In detail, $\hat{E_1}$ has $AUC = 0.67574$ while $AUC = 0.74338$ for $\hat{E_2}$.(Under 50-times iterations setting). Moreover, for $p = 100$ and $n = 200$, which corresponds to the ratio $\frac{p}{n} = 2$, ROC curve(*Figure 2.3.2.4*) is plotted. $\hat{E_1}$ has $AUC = 0.43343$ while $AUC = 0.59768$ for $\hat{E_2}$.

Figure 2.3.2.2

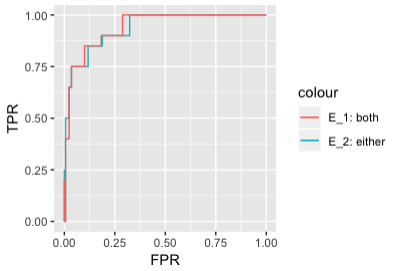


Figure 2.3.2.3

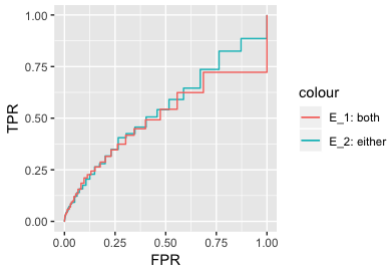
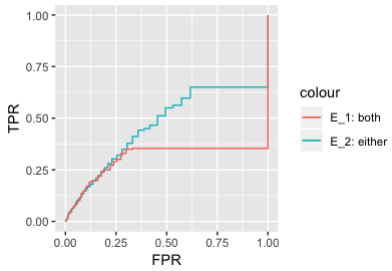


Figure 2.3.2.4



In conclusion, by conducting more simulations on different $\frac{p}{n}$ settings, *Table 2.3.2.5* is generated to show all the outcomes. **Obviously, by increasing the $\frac{p}{n}$ ratio from 0.02 to 2, Both $\hat{E_1}$ and $\hat{E_2}$ had their performance decreased over the ratio.** When $\frac{p}{n} = 0.02$, both methods achieved impressive performace which is larger than $AUC = 0.99$. In the $n = p$ situation, Both methods perform worse than the last case, while $\hat{E_1}$'s AUC decreases 31.88% and AUC decreases 25.02% for $\hat{E_2}$ from $\frac{p}{n} = 0.02$ case. In the end, if $\frac{p}{n} = 2$, we can see that $AUC(\hat{E_1})$ dropped below 0.5 for the first time, while $AUC(\hat{E_2})$ still higher than 0.5.

Vertically, **under each $\frac{p}{n}$ setting, $\hat{E_2}$ will usually achieve better result than the $\hat{E_1}$**, although both of the methods perform very well in $\frac{p}{n} = 0.02$, in which big enough data allows lasso and linear regression to inference the hidden structure of the edge set. Similarly, both methods perform not well in the setting $\frac{p}{n} = 2$, in which "lack of data" leads to this outcome.