

The `huge` Package for High-dimensional Undirected Graph Estimation in R

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Abstract

We describe an R package named `huge` which provides easy-to-use functions for estimating high dimensional undirected graphs from data. This package implements recent results in the literature, including Friedman et al. [2007b], Liu et al. [2009] and Liu et al. [2010]. Compared with the existing graph estimation package `glasso`, the `huge` package provides extra features: (1) instead of using Fortran, it is written in C, which makes the code more portable and easier to modify; (2) besides fitting Gaussian graphical models, it also provides functions for fitting high dimensional semiparametric Gaussian copula models; (3) more functions like data-dependent model selection, data generation and graph visualization; (4) a minor convergence problem of the graphical lasso algorithm is corrected; (5) the package allows the user to apply both lossless and lossy screening rules to scale up large-scale problems, making a tradeoff between computational and statistical efficiency.

1 Overview

Undirected graphs is a natural approach to describe the conditional independence among many variables. Each node of the graph represents a single variable and no edge between two variables implies that they are conditional independent given all other variables.

In the past decade, significant progress has been made on designing efficient algorithms to learn undirected graphs from high-dimensional observational datasets. Most of these

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methods are based on either the penalized maximum-likelihood estimation [Friedman et al., 2007b] or penalized regression methods [Meinshausen and Bühlmann, 2006]. Existing packages include `glasso`, `Covpath`, `CLIME` and `parcor`. In particular, the `glasso` package has been widely adopted by statisticians and computer scientists due to its friendly user-inference and efficiency. There are also other graph estimation packages such as `GeneNet` and `sna`, but they are not targeting on conditional independence graph estimation.

In this vignette, we describe a newly developed R package named `huge` (High-dimensional Undirected Graph Estimation). Compared with `glasso`, the core engine of `huge` is coded in C, making modifications of the package more accessible to researchers from the computer science and signal processing communities. The package includes a wide range of functional modules, including data generation, data preprocessing, graph estimation, model selection, and visualization. Many recent methods have been implemented, including the nonparanormal [Liu et al., 2009] method for estimating a high dimensional Gaussian copula graph, the StARS [Liu et al., 2010] approach for stability-based graphical model selection, and correlation screening [Fan and Lv, 2008] for graph estimation. The package supports two modes of screening, lossless [Witten et al., 2011, Mazumder and Hastie, 2011a] and lossy screening. The user can select the desired screening level to scale up to larger problems, but this introduces some estimation bias. This package also addresses some minor convergence problem of the graphical lasso algorithm.

2 Background

2.1 Gaussian Graphical Models

The Gaussian Graphical Models assumes that the observations have a multivariate Gaussian distribution with mean μ , and covariance matrix Σ . The conditional independence can be implied by the inverse covariance (concentration) matrix $\Omega = \Sigma^{-1}$. If $\Omega_{jk} = 0$, then the i -th variable and j -th variables are conditional independent given all other variables. Thus it makes sense to impose an ℓ penalty for the estimation of Ω , to increase its sparsity, and the sparse pattern of Ω is essentially the same as the adjacency matrix of the underlying undirected graph.

Meinshausen and Bühlmann [2006] take a simple approach to this problem and they estimate a sparse graphical model by the following minimization problem,

$$\hat{\mathcal{G}} = \underset{\mathcal{G} \in \mathbb{R}^{d \times d}, \mathcal{G}_{jj} = 0}{\operatorname{argmin}} \frac{1}{2} \operatorname{Tr}(\mathcal{G}^T S \mathcal{G}) - \operatorname{Tr}(\mathcal{G}^T S) + \lambda \|\mathcal{G}\|_1 \text{ for all } j = 1, \dots, d \quad (1)$$

where S denotes the sample covariance matrix and $\lambda > 0$ is the regularization parameter controlling the sparsity level. (2.1) is equivalent to fitting lasso to each variable, using the others as predictors. The component $\hat{\Omega}_{ij}$ is then estimated to be non-zero if either the

estimated coefficient of variable i on j , $(\widehat{\mathcal{G}}_{ij})$, or the estimated coefficient of variable j on i , $(\widehat{\mathcal{G}}_{ji})$, is non-zero (alternatively they use an AND rule), i.e. $\widehat{\mathcal{G}}$ has the same sparse pattern as $\widehat{\Omega}$. They show that asymptotically, this consistently estimates the sparse pattern of Ω .

Other authors have proposed algorithms for the exact maximization of the ℓ_1 -penalized log-likelihood and also formulates the estimation of Ω as a convex minimization problem,

$$\widehat{\Omega} = \underset{\Omega \in \mathbb{R}^{d \times d}, \Omega \succ 0}{\operatorname{argmax}} \log |\Omega| - \operatorname{Tr}(\Omega^T S) - \lambda \|\Omega\|_1 \quad (2)$$

Banerjee et al. [2008] establish that the simpler approach of Meinshausen and Bühlmann [2006] can be viewed as an approximation to the exact problem. While (2) can numerically estimate Ω , which usually leads to more possible applications.

In our implementation of the package `huge`, we exploit many suggested tricks and practices from Friedman et al. [2007b,a, 2010a]. We solve using coordinate descent and (2) using block coordinate descent. They are both combined with active set and covariance update tricks. We also modify the warm start trick to address the potential divergence problem of the graphical lasso algorithm [Mazumder and Hastie, 2011b].

Remark 1. *Meinshausen and Bühlmann [2006] is more efficient than Banerjee et al. [2008] in computation, but the degrees of nodes for the estimation are usually restricted, since we cannot get the non-zeros entries more than the sample size in each ℓ_1 -regularized regression problem.*

Remark 2. *Both Meinshausen and Bühlmann [2006] and Banerjee et al. [2008] can asymptotically recover the true sparsity pattern under the irrerepresentable condition and a suitable choice of regularization. When the condition is violated or the regularization parameter is not well tuned, it is highly difficult to achieve perfect recovery.*

2.2 Gaussian Copula Models

Gaussian copula models extends the Gaussian graphical models by marginally transforming the variables using smooth monotone functions. The underlying distribution is still assumed to be d -variate Gaussian distribution $N(0, \Sigma)$ by introducing a collection of monotone functions f_j 's such that $(f_1(X_1), \dots, f_d(X_d))^T \sim N(0, \Sigma)$. The primary goal of the nonparanormal is to estimate the underlying sample covariance matrix for a better recovery of the underlying undirected graph [Liu et al., 2009].

Suppose we have n observations for j -th variable, x_{1j}, \dots, x_{nj} , we sort all n observations and get the corresponding rank u_{1j}, \dots, u_{nj} . Let Φ denote the Gaussian CDF function,

then we can estimate the transformed data using:

$$\underbrace{\hat{f}_j(x_{ij}) = \Phi^{-1}(\hat{u}_{ij})}_{\text{The normal score}} \text{ or } \underbrace{\hat{f}_j(x_{ij}) = \begin{cases} \Phi^{-1}(\delta) & \text{if } \hat{u}_{ij} \leq \delta \\ \Phi^{-1}(\hat{u}_{ij}) & \text{if } \delta < \hat{u}_{ij} \leq 1 - \delta \\ \Phi^{-1}(1 - \delta) & \text{if } \hat{u}_{ij} > 1 - \delta \end{cases}}_{\text{The truncated normal}} \quad (3)$$

where

$$\hat{u}_{ij} = \frac{u_{ij}}{n+1} \text{ and } \delta = \frac{1}{4n^{1/4}\sqrt{\pi \log n}}. \quad (4)$$

2.3 Screening

Although efficient algorithms have been developed, it is still very difficult to efficiently solve large scale problem. In the past few years, several fast screening method have been proposed to address the fast pre-selection before graph estimation. They aim to first reduce the high dimension to the moderate size with the informative variables preserved. Then the refined algorithm can be further applied.

In our implementation, we provide an optional procedure Fan and Lv [2008] to Meinshausen and Bühlmann [2006]. In each lasso problem, we can select the variables having larger sample correlation with the response. Since Fan and Lv [2008] only guarantee under certain regularity condition, it can preserve the informative variables with a large probability. We refer it as the lossy screening rule.

We further extended Fan and Lv [2008] to Friedman et al. [2007b]. If $S_{ij} \leq \lambda$, then we will set no edge between the i -th and j -th variable. In fact the graph generated by our lossy screening based on correlation can also roughly approximate the underlying partial correlation graph Friedman et al. [2010a]. Due to its low computational cost, it has been widely applied in biomedical research [Langfelder and Horvath, 2008].

Witten et al. [2011], Mazumder and Hastie [2011b] also establish a very simple rule to pre-select the nodes before graph estimation. If $S_{ij} \leq \lambda$ for all $j \neq i$, then the i -th variable will be a isolated node in the final estimator. Eventually we only need to estimate a small block of the inverse covariance matrix. This screening rule is derived from the perspective of convex optimization (KKT condition), and doesn't affect the statistical efficacy. We refer it to the lossless screening rule.

3 Design and Implementation

The package `huge` aims to provide a general framework for high-dimensional undirected graph estimation. Six functional modules (M1-M6) facilitate a flexible pipeline for analysis (Figure 1).

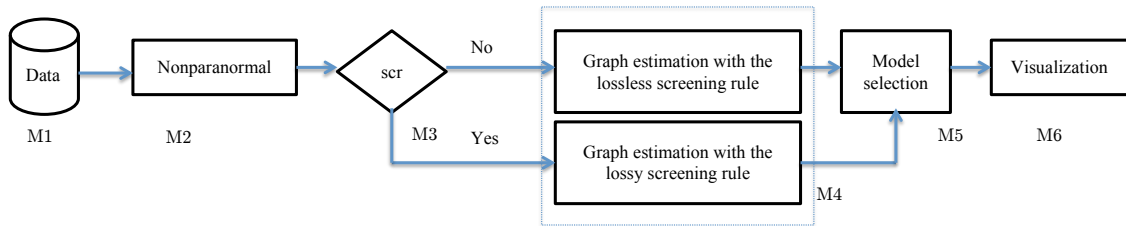


Figure 1: The graph estimation pipeline.

M1. Data Generator: The function `huge.generator()` can generate multivariate Gaussian data with different undirected graph structures, including hub, cluster, band, scale-free, and Erdős-Rényi random graphs. The sparsity level of the graph structures and signal-to-noise ratios can also be adjusted by users.

M2. Semiparametric Transformation: The function `huge.npn()` implements the nonparanormal method [Liu et al., 2009] for estimating a semiparametric Gaussian copula model by truncated normal or normal score. Computationally, the estimation of a nonparanormal transformation only requires one pass through the data matrix.

Remark 3. *Although in the existing high-dimensional theory, the truncation has been proved to be asymptotically consistent and no corresponding result has been established for normal score, we find the normal score also has a good performance in practice.*

M3. Graph Screening: The `scr` argument in the main function `huge()` controls the use of large-scale correlation screening before graph estimation. The function supports two types of screening rules, lossless screening and lossy screening. The lossless screening method is from Witten et al. [2011], Mazumder and Hastie [2011b] and the lossy screening method is from Fan and Lv [2008]. Such screening procedures can greatly reduce the computational cost and achieve equal or even better estimation by reducing the variance at the expense of an increase in bias.

M4. Graph Estimation: Similar to the `glasso` package, the `method` argument in the `huge()` function supports two estimation methods: (i) the Meinshausen-Bühlmann covariance selection algorithm [Meinshausen and Bühlmann, 2006] and (ii) the graphical lasso algorithm [Friedman et al., 2007b, Banerjee et al., 2008]. One difference between `huge` and `glasso` is that we implement all the core components using C instead of Fortran. The code is also memory-optimized using sparse matrix data structures so that it can handle larger datasets when estimating and storing full regularization paths. We also provide an additional graph estimation method based on thresholding the sample correlation matrix. Such an approach is computationally efficient and has been widely applied in biomedical research [Langfelder and Horvath, 2008].

Remark 4. *We find the graphical lasso algorithm may fail to converge using the warm start trick when estimating the solution path. We proposed a modified warm start trick and explained the reason of the failure for the original warm start trick in the Appendix.*

M5. Model Selection: The function `huge.select()` provides three regularization parameter selection methods: the stability approach for regularization selection (StARS) [Liu et al., 2010]; a modified rotation information criterion (RIC) [Lysen, 2009]; and the extended Bayesian information criterion [Foygel and Drton, 2010]. The latter approach is a likelihood-based model selection criterion that is only applicable for the graphical lasso method. StARS conducts many subsampling steps to calculate variability score using the U-statistics, which is computationally intensive but can be trivially parallelized. RIC is closely related to the permutation approach for model selection and scales to large datasets.

Remark 5. *Under certain regularity condition, StARS is partially consistent and suffers overselection. The performance of StARS also depends on the tuning grid chosen by user.*

Remark 6. *RIC randomly rotates the variables for each sample multiple times and selects the minimum regularization which generates all zero estimated using rotated data. It has no theoretical guarantee of the consistent recovery and often suffers serious underselection or overselection.*

M6. Graph Visualization: The plotting functions `huge.plot()` and `plot()` provide visualizations of the simulated data sets, estimated graphs and paths. The implementation is based on the `igraph` package. Due to the limits of `igraph`, sparse graphs with only up to 2,000 nodes can be visualized.

4 User Interface by Example

We illustrate the user interface by two simple examples. The first one is based on the simulated data generated by `huge.generator()`,

```
> library(huge) # Load the package huge
> L = huge.generator(n=200,d=200,graph="hub") # Generate data with hub structures
> X = L$data; X.pow = X^3/sqrt(15) # Power Transformation
> X.npn = huge.npn(X.pow) # Nonparanormal
> out.mb = huge(X.pow,nlambda=30) # Estimate the solution path
> out.npn = huge(X.npn,nlambda=30)
> huge.roc(out.mb$path,L$theta) # Plot the ROC curve
> huge.roc(out.npn$path,L$theta)
> mb.stars = huge.select(out.mb,criterion="stars",
+ stars.thresh=0.05) # Select the graph using StARS
> npn.stars = huge.select(out.npn,criterion="stars",stars.thresh=0.05)
> mb.ric = huge.select(out.mb) # Select the graph using RIC
> npn.ric = huge.select(out.npn)
```

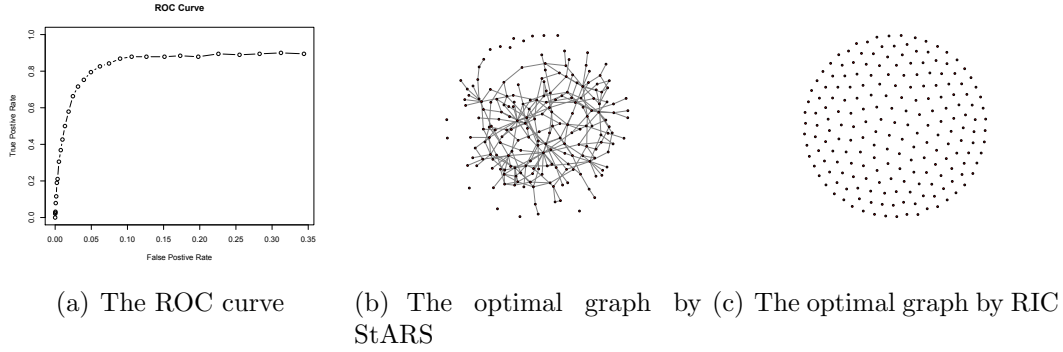


Figure 2: Simulated results w/o nonparanormal

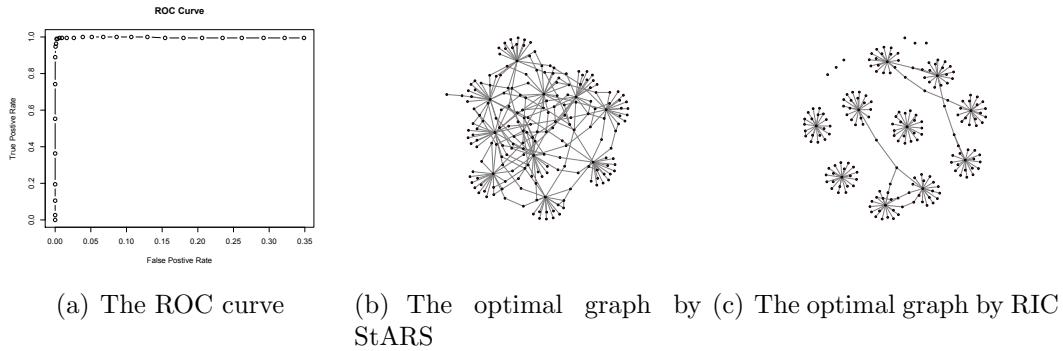


Figure 3: Simulated results w/ nonparanormal

We generate 200 samples following a 200-dimensional Gaussian distribution with the hub structure, then transform the data using power transformation, which preserves the population mean and population variance. The graph is estimated by Meinshausen and Bühlmann [2006] by default. The program automatically sets up a sequence of 30 regularization parameters and estimates the corresponding graph path. The results w/o and w/ non paranormal are shown in Figure 2 and Figure 3 respectively. We can see a significant improvement by using nonparanormal. As mentioned in the previous section, the StARS and RIC yields a overselected and a underselected graph respectively.

The second example is based on a stock market data which we contribute to the `huge` package. We acquired closing prices from all stocks in the S&P 500 for all the days that the market was open between January 1, 2003 and January 1, 2008. This gave us 1258 samples for the 452 stocks that remained in the S&P 500 during the entire time period.

```
> data(stockdata) # Load the stock data
> Y = log(stockdata$data[2:1258,]/stockdata$data[1:1257,]) # Preprocessing
```

Here the data have been transformed by calculating the log-ratio of the price at time t to price at time $t - 1$, and then standardized by subtracting the mean and adjusting the variance to one.

```
> Y.npn = huge.npn(Y, npn.func="truncation") # Nonparanormal
```

```
> out.npn = huge(Y.npn,method = "glasso", nlambda=40,lambda.min.ratio = 0.4)
> out = huge(Y,method = "glasso", nlambda=40,lambda.min.ratio = 0.4)
```

Here the nonparanormal transformation is applied to the data, and the graph is estimated using the graphical lasso (the default is the Meinshausen-Bühlmann estimator). The program automatically sets up a sequence of 40 regularization parameters and estimates the corresponding graph path. The lossless screening method is applied by default. The output of graph estimation using the transformed data is shown in Figure 4. To investigate

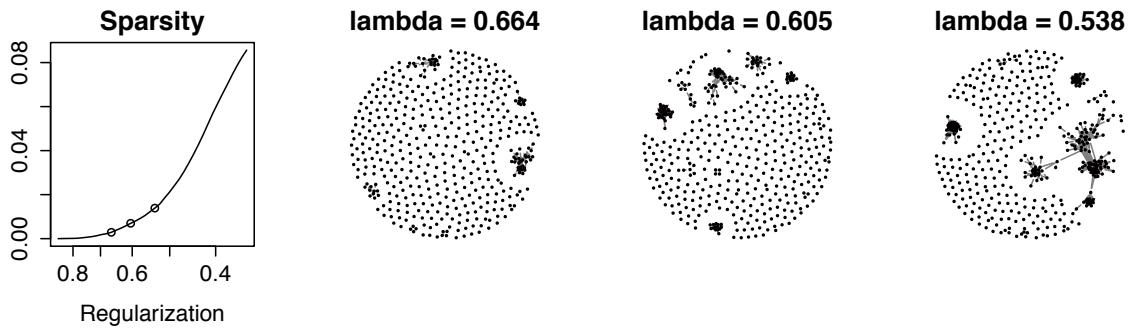


Figure 4: The estimated graph path.

the impact of the nonparanormal transformation, we plot points in a subgraph calculated with and without the transformation (Figure 5). Both graphs have the sparsity level at

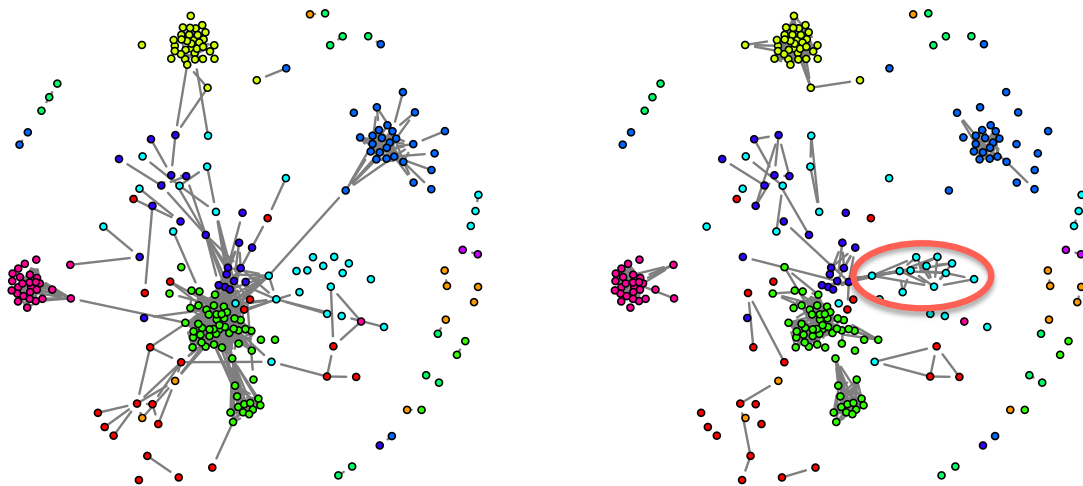


Figure 5: The estimated glasso graph (left) and nonparanormal graph (right).

about 1% and we can see the different pattern between them. We highlight a dense module in the nonparanormal graph which is much sparser in the corresponding glasso graph. We can see all nodes in this module belong to the same category. This example well demonstrates the power of the nonparanormal method to reveal the relationship beyond the normality assumption.

5 Performance Benchmark

We adopt similar experimental settings as in Friedman et al. [2010b] to compare **huge** with **glasso** (ver 1.4). We consider four scenarios with varying sample sizes n and number of variables d , as shown in Table 1. We simulate the data from three different multivariate normal distributions with null graph (diagonal covariance matrix) and Erdős-Rényi random graph (with probability 0.01) structures respectively. Timings (in seconds) are computed over 10 values of the corresponding regularization parameter, and the range of regularization parameters is chosen so that each method produced approximately the same number of non-zero estimates. The convergence threshold of both **glasso** and **huge** is chosen to be 10^{-4} . All experiments were carried out on a PC with Intel Core i5 3.3GHz processor. Unfortunately, **CLIME** (ver 1.0) **Covpath** (ver 0.2), were unable to obtain timing results due to numerical issues. **parcor** (ver 0.22) failed to get any results in 3 hours.

Table 1: Experimental Results on Null Graph

Method	$d = 1000$ $n = 100$	$d = 2000$ $n = 150$	$d = 3000$ $n = 200$	$d = 4000$ $n = 300$
huge -Meinshausen-Bühlmann (lossy)	2.688 (0.140)	11.14 (0.623)	30.47 (0.738)	223.5 (13.14)
huge -Meinshausen-Bühlmann	4.032 (0.267)	37.51 (2.254)	119.6 (3.888)	330.6 (25.49)
glasso -Meinshausen-Bühlmann	34.38 (0.481)	245.8 (4.143)	800.7 (7.652)	2694 (136.5)
huge -graphical lasso (lossy)	34.39 (2.173)	246.5 (16.18)	857.3 (24.18)	2015 (151.1)
huge -graphical lasso (lossless)	43.13 (3.461)	310.4 (28.19)	1071 (41.51)	2510 (293.4)
glasso -graphical lasso	122.1 (5.259)	931.4 (45.96)	2998 (97.71)	7485 (307.5)

For Meinshausen-Bühlmann graph estimation, we can see that **huge** achieves the best performance. In particular, when the lossy screening rule is applied, **huge** automatically reduces each individual lasso problem from the original dimension d to the sample size n , therefore even better efficiency can be achieved in settings when $d \gg n$. Based on our experiments, the speed up due to the lossy screening rule can be up to 400%.

Table 2: Experimental Results on Random Graph

Method	$d = 1000$ $n = 100$	$d = 2000$ $n = 150$	$d = 3000$ $n = 200$	$d = 4000$ $n = 300$
huge -Meinshausen-Bühlmann (lossy)	3.246 (0.147)	13.47 (0.665)	35.87 (0.97)	247.2 (14.26)
huge -Meinshausen-Bühlmann	4.24 (0.288)	42.41 (2.338)	147.9 (4.102)	357.8 (28.00)
glasso -Meinshausen-Bühlmann	37.23 (0.516)	296.9 (4.533)	850.7 (8.180)	3095 (150.5)
huge -graphical lasso (lossy)	39.61 (2.391)	289.9 (17.54)	905.6 (25.84)	2370 (168.9)
huge -graphical lasso (lossless)	47.86 (3.583)	328.2 (30.09)	1276 (43.61)	2758 (326.2)
glasso -graphical lasso	131.9 (5.816)	1054 (47.52)	3463 (107.6)	8041 (316.9)

Unlike the Meinshausen-Bühlmann graph approach, the graphical lasso estimates the inverse covariance matrix. The lossless screening rule [Witten et al., 2011, Mazumder and Hastie, 2011b] greatly reduces the computation required by the graphical lasso algorithm, especially when the estimator is highly sparse. The lossy screening rule can further speed up the algorithm and provides an extra performance boost.

6 Conclusions

We developed a new package named `huge`, for high dimensional undirected graph estimation. The package is complementary to the existing `glasso` package by providing extra features and functional modules. We plan to maintain and support this package in the future.

7 Appendix

7.1 A Typical Example of Failure

In the package `glasso`, the warm start trick begins with the larger regularization parameters and gradually decreases the regularization parameter. However, in real applications, we find this strategy may lead to divergence or other numerical issues sometimes. We first provide an example that `glasso` fails to converge.

```
> library(huge) # load the package huge
> library(glasso) # Load the package glasso
> data(stockdata) # Load the stock data
> X = log(stockdata$data[2:1258,]/stockdata$data[1:1257,]) # Preprocessing
> out.huge = huge(X,method = "glasso", nlambda=5)
> out.glasso = glassopath(cor(X),rholist = out.huge$lambda[5:1])
```

7.2 A Modified Warm Start trick

From Banerjee et al. [2008], we know a good initial value for the estimated covariance matrix $\widehat{\Sigma}$ should satisfy the constraint

$$\|\widehat{\Sigma} - S\|_{\infty} \leq \lambda \text{ and } \Sigma \succ 0 \quad (5)$$

where S is the sample covariance matrix. Otherwise, the algorithm cannot guarantee the positive definiteness of the estimation. Once the positive definiteness is violated in some iteration, the whole algorithm will fail. Now suppose we have a sequence of decreasing regularization parameters $\lambda_1, \dots, \lambda_K$ and for λ_k , we have obtain the estimated covariance matrix as $\widehat{\Sigma}_k$. By KKT condition, we know

$$\|\widehat{\Sigma}_k - S\|_{\infty} \leq \lambda_k \quad (6)$$

However, when we use $\widehat{\Sigma}_k$ as the initial values for estimating $\widehat{\Sigma}_{k+1}$ corresponding to λ_{k+1} , although $\widehat{\Sigma}_k \succ 0$ hold, it is highly likely that $\widehat{\Sigma}_k$ may violate our requirement of (5) when using the regularization parameter λ_{k+1} , since $\lambda_k > \lambda_{k+1}$. The glass algorithm may tolerate slight violation sometimes, but when we decrease the regularization parameter

too fast, then a failure is highly likely to happen. The phenomenon was also found independently by Mazumder and Hastie [2011b].

In our implementation of the graphical lasso, we actually take the initial covariance matrix as the sample covariance matrix and compute the path using the regularization parameters in the increasing order. We sacrifice a little bit efficiency, but guarantee our **huge** won't fail due to the warm start trick. Although our strategy is quite counterintuitive, but it works well in practice. In the previous example, **huge** successfully estimated the solution path for only seconds, while **glasso** showed no intent to stop, thus we killed the corresponding process after 3 hours.

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