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

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Abstract

We describe an R package called huge (ver 1.2), that provides easy-to-use functions for estimating high dimensional undirected graphs from data. This package implements recent results in the literature, including Meinshausen and Bühlmann [2006], Friedman et al. [2007b], Liu et al. [2009] and Liu et al. [2010]. Compared with the existing package glasso, the huge package provides several extra features: (i) instead of using Fortran, it is written in C, which makes the code more portable and easier to modify; (ii) besides fitting Gaussian graphical models, it also provides functions for fitting high dimensional semiparametric Gaussian copula models, data-dependent model selection, data generation and graph visualization; and (iii) to achieve better scalability, it incorporates correlation screening into graph estimation. In particular, the package allows the user to apply both lossless and lossy screening rules to scale up for high-dimensional problems, making a tradeoff between computational and statistical efficiency.

1 Overview

Significant progress has been made recently on designing efficient algorithms to learn undirected graphical models from high-dimensional observational datasets. Existing packages include glasso [Friedman et al., 2007b], Covpath [Krishnamurthy and d'Aspremont, 2011] and CLIME [Cai et al., 2010]. In particular, the glasso package has been widely adopted by statisticians and computer scientists due to its friendly user-inference and efficiency. In this paper, 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.

2 Gaussian Graphical Models and Copula Models

2.1 Gaussian Graphical Models

In Gaussian Graphical Models, $X = (X_1, ..., X_d)^T$ is assumed to follow a d-variate Gaussian distribution $N(0, \Sigma)$. The conditional independence can be obtained by the inverse covariance

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[¶]email: larry@stat.cmu.edu, Department of Statistics, Carnegie Mellon University (concentration) matrix $\Omega = \Sigma^{-1}$ and $\Omega_{jk} = 0$ means that the i-th variable and j-th variables are conditional independent given all other variables. The sparse pattern of Ω can also be represented in a undirected graph, therefore estimating a Gaussian Graphical Models is usually referred to undirected graph estimation.

Meinshausen and Bühlmann [2006] only estimates the sparse pattern Ω by solving a collection of ℓ_1-regularized regression problems,

$$\hat{\beta} = \underset{\beta \in \mathbb{R}^d, \beta_j = 0}{\operatorname{argmin}} \frac{1}{2}\beta^T S \beta - S_j \beta + \lambda \|\beta\|_1 \text{ for all } j = 1, ..., d \tag{1}$$

where S denotes the sample covariance matrix Σ_j denotes the j-th row of Σ, and $\lambda > 0$ is the regularization parameter controlling the sparsity level. Each $\hat{\beta}$ corresponds to a column in $\hat{\Omega}$ in term of the sparsity pattern.

Banerjee et al. [2008] directly formulates the estimation of Ω as a ℓ_1 penalized maximum likelihood problem,

$$\widehat{\Omega} = \underset{\Omega \in \mathbb{R}^{d \times d}, \Omega \succ 0}{\operatorname{argmax}} \log |\Omega| - \langle S, \Omega \rangle - \lambda \|\Omega\|_1 \tag{2}$$

(2) can numerically estimate Ω, which usually leads to more possible applications.

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 nonzeros 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 irrepresentable condition. When the condition is violated, 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 $N(0, \Sigma)$ and there exists a collection of monotone functions f_j's such that $(f_1(X_1), ..., f_d(X_d))^T \sim N(0, \Sigma)$. 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]. Gaussian Copula models is applicable to not only continuous data but also discrete data.

Suppose we have n observations for j-th variable, $x_{1j}, ..., x_{nj}$, we sort all n observations and get the corresponding rank $u_{1j}, ..., u_{nj}$. Let Φ denote the Gaussian CDF function, then we can estimate the transformed data using:

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

where

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

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

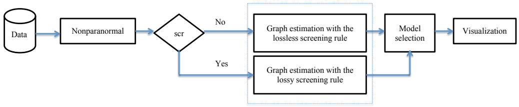

Data
Nonparanormal
scr
No
Yes
Graph estimation with the lossless screening rule
Graph estimation with the lossy screening rule
Model selection
Visualization

Figure 1: The graph estimation pipeline.

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]. In our implementation, we exploit many suggested tricks and practices from Friedman et al. [2007b,a, 2010a]. For example, we solve each individual lasso problem using coordinate descent combined with active set and covariance update tricks. 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.*

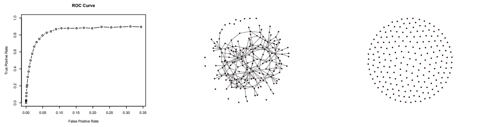
Remark 6. *RIC randomly rotates the variables for each sample multiple times and selects the minimum regularization which generates all zero estimated using rotated data. It has no theoretical guarantee of the consistent recovery and often suffers serious underselection or overselection.*

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

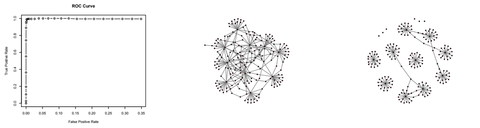
We illustrate the user interface by two simple examples. The first one is based on the simulated data generated by huge.generator(),

```
> 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)
```



(a) The ROC curve (b) The optimal graph by StARS (c) The optimal graph by RIC

Figure 2: Simulated results w/o nonparanormal



(a) The ROC curve (b) The optimal graph by StARS (c) The optimal graph by RIC

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 tend to 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 the impact of the nonparanormal

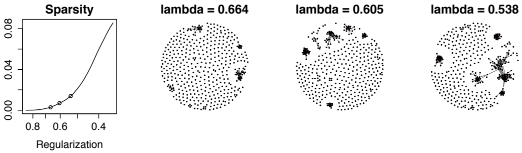


Figure 4: The estimated graph path.

transformation, we plot points in a subgraph calculated with and without the transformation (Figure 5). Both graphs have the sparsity level at about 1% and we can see the different pattern

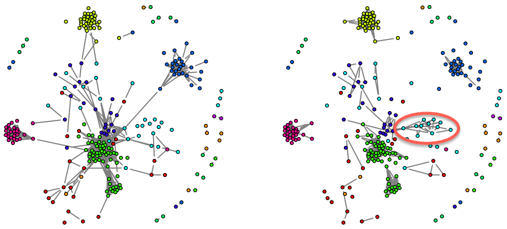


Figure 5: The estimated glasso graph (left) and nonparanormal graph (right).

between them. We highlight a dense module in the nonparanormal graph which is much sparser in the corresponding glasso graph.

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 Erdös-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 and 8GB memory. We also tried CLIME (ver 1.0) and Covpath (ver 0.2), but were unable to obtain timing results due to numerical issues.

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 screening)	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 screening)	34.39 (2.173)	246.5 (16.18)	857.3 (24.18)	2015 (151.1)
huge-graphical lasso (lossless screening)	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 screening)	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 screening)	39.61 (2.391)	289.9 (17.54)	905.6 (25.84)	2370 (168.9)
huge-graphical lasso (lossless screening)	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

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

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 $\lambda_1, ..., \lambda_K$ and for λ_k, we have obtain the estimated covariance matrix as $\widehat{\Sigma}_k$. By KKT condition, we know

$$\|\widehat{\Sigma}_k - S\|_{\infty} \leq \lambda_k \tag{6}$$

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` successful 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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