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

Tuo Zhao
Han Liu
Johns Hopkins University
Baltimore, MD 21218, USA

Kathryn Roeder
John Lafferty
Larry Wasserman
Carnegie Mellon University
Pittsburgh, PA, 15213

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Abstract
We describe an R package called huge (ver 1.1.2), that provides easy-to-use functions for estimating high dimensional undirected graphs from data. This package implements recent results in the literature, including Friedman et al. (2007), Liu et al. (2009) and Liu et al. (2010). Compared with 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.

Keywords: high-dimensional undirected graph estimation, glasso, huge, semiparametric graph estimation, data-dependent model selection, lossless screening, lossy screening.

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., 2007], Covpath and CLIME. 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 im-

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implemented, including the nonparanormal \cite{liu2009} for estimating a high dimensional Gaussian copula graph, the StARS \cite{liu2010} approach for stability-based graphical model selection, and correlation screening for high dimensional graph estimation. The package supports two modes of screening, lossless \cite{witten2011} and lossy screening. When using lossy screening, the user can select the desired screening level to scale up for high-dimensional problems, but this introduces some estimation bias.

2. Design and Implementation

The package \texttt{huge} aims to provide a general framework for high-dimensional undirected graph estimation. The package includes six functional modules (M1-M6), see (Figure 1).

![Figure 1: The graph estimation pipeline.](image)

**M1. Data Generator:** The function \texttt{huge.generator()} can simulate multivariate Gaussian data with different undirected graph structures, including hub, cluster, band, scale-free, and Erdős-Rényi random graphs. The sparsity level of the obtained graph and signal-to-noise ratio can also be set up by users.

**M2. Semiparametric Transformation:** The function \texttt{huge.npn()} implements the nonparanormal method \cite{liu2009} for estimating a semiparametric Gaussian copula model. Motivated by additive models, the nonparanormal family extends the Gaussian distribution by marginally transforming the variables using smooth functions. Computationally, the nonparanormal transformation only requires one pass through the data matrix.

**M3. Graph Screening:** The \texttt{scr} argument in the main function \texttt{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 \cite{witten2011}. Such screening procedures can greatly reduce the computational cost and achieve equal or even better estimation by reducing the variance at the expense of increased bias.

**M4. Graph Estimation:** Similar to the \texttt{glasso} package, the \texttt{method} argument in the \texttt{huge()} function supports two estimation methods: (i) the Meinshausen-Bühlmann covariance selection algorithm \cite{meinshausen2006} and (ii) the graphical lasso algorithm \cite{friedman2007}. In our implementation, we exploit many suggested tricks and practices from \cite{friedman2010a}. For example, we solve each individual lasso problem using coordinate descent combined with active set and covariance update tricks. One difference between \texttt{huge} and \texttt{glasso} is that we implement all the core components using \texttt{C} instead of \texttt{Fortran}. The code is also memory-optimized using the sparse matrix data structure 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.
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); and the extended Bayesian information criterion. 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 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.

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.

3. User Interface by Example

We illustrate the user interface by analyzing 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 Jan 1, 2003 and Jan 1, 2008. This gave us 1258 samples for the 452 stocks that remained in the S&P 500 during the entire time period.

```r
> library(huge)
> data(stockdata) # Load the data
> x = log(stockdata$data[2:1258,]/stockdata$data[1:1257,]) # Preprocessing
> x.npn = huge.npn(x, npn.func="truncation") # Nonparanormal
> out.npn = huge(x.npn, method = "glasso", nlambda=40, lambda.min.ratio = 0.4)
```

Here the data have been transformed by calculating the log-ratio of the price at time $t$ to price at time $t-1$. The nonparanormal transformation is applied to the data, and a 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 graph path. The lossless screening method is applied by default.

4. 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 dimensionality $d$, as shown in Table 1. We simulate the data from a normal distribution $N(0, I_d)$. 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 sparsity level is from 0 to about 0.03). 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 3.3Hz processor. We also tried CLIME (ver 1.0) and Covpath (ver 0.2), but were unable to obtain timing results due to numerical issues.

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

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2. We thank Mladen Kolar for providing the python code to crawl the data from the web.
reduces each individual lasso problem from the original dimension $d$ to the sample size $n$, therefore a 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 500%.

Unlike the Meinshausen-Bühlmann graph approach, the graphical lasso estimates the inverse covariance matrix. The lossless screening rule (Witten and Friedman, 2011) 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.

5. Summary

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.

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