Composite likelihood estimation of sparse Gaussian graphical models with symmetry

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ABSTRACT

In this article, we discuss the composite likelihood estimation of sparse Gaussian graphical models. When there are symmetry constraints on the concentration matrix or partial correlation matrix, the likelihood estimation can be computational intensive. The composite likelihood offers an alternative formulation of the objective function and yields consistent estimators. When a sparse model is considered, the penalized composite likelihood estimation can yield estimates satisfying both the symmetry and sparsity constraints and possess ORACLE property. Application of the proposed method is demonstrated through simulation studies and a network analysis of a biological data set.

Key words: Variable selection; model selection; penalized estimation; Gaussian graphical model; concentration matrix; partial correlation matrix

1. Introduction

A multivariate Gaussian graphical model is also known as covariance selection model. The conditional independence relationships between the random variables are equivalent to specified zeros among the inverse covariance matrix. More exactly, let $X = (X^{(1)}, ..., X^{(p)})$ be a p-dimensional random vector following a multivariate normal distribution $N_p(\mu, \Sigma)$, with μ denoting the unknown mean and Σ denoting the nonsingular covariance matrix. Denote the inverse covariance matrix as $\Sigma^{-1} = C = (C_{ij})_{1 \le i,j \le p}$. Zero entries C_{ij} in the inverse covariance matrix indicate conditional independence between the random variables $X^{(i)}$ and $X^{(j)}$ given all other variables (Dempster (1972), Whittaker (1990), Lauritzen (1996)). The Gaussian random vector X can be represented by an undirected graph $G = (V, E)$, where V contains p vertices corresponding to the p coordinates and the edges $E = (e_{ij})_{1 \le i < j \le p}$ represent the conditional dependency relationships between variables $X^{(i)}$ and $X^{(j)}$. It is of interest to identify the correct set of edges, and estimate the parameters in the inverse covariance matrix simultaneously.

To address this problem, many methods have been developed. In general, there are no zero entries in the maximum likelihood estimate, which results in a full graphical structure. Dempster (1972) and Edwards (2000) proposed to use penalized likelihood with the L_0-type penalty $p_\lambda(|c_{ij}|)_{i \neq j} = \lambda I(|c_{ij}| \neq 0)$, where $I(.)$ is the indicator function. Since the L_0 penalty is discontinuous, the resulting penalized likelihood estimator is unstable. Another approach is stepwise forward selection or backward elimination of the edges. However, this ignores the stochastic errors inherited in the multiple stages of the procedure (Edwards (2000)) and the statistical properties of the method are hard to comprehend. Meinshausen and Bühlmann (2006) proposed a computationally attractive method for covariance selection; it performs the neighborhood selection for each node and combines the results to learn the overall graphical structure. Yuan and Lin (2007) proposed penalized likelihood methods for estimating the concentration matrix with the L_1 penalty (LASSO) (Tibshirani (1996)). Banerjee, Ghaoui, and D'aspremont (2007) proposed a block-wise updating algorithm for the estimation of the inverse covariance matrix. Further in this line, Friedman, Hastie, and Tibshirani (2008) proposed the graphical LASSO algorithm to estimate the sparse inverse covariance matrix using the LASSO penalty through a coordinate-wise updating scheme. Fan, Feng, and Wu (2009) proposed to estimate the inverse covariance matrix using the adaptive LASSO and the Smoothly Clipped Absolute Deviation (SCAD) penalty to attenuate the bias problem. Friedman, Hastie and Tibshirani (2012) proposed to use composite likelihood based on conditional likelihood to estimate sparse graphical models.

In real applications, there often exists symmetry constraints on the underlying Gaussian graphical model. For example, genes belong to the same functional or structure group may behave in a similar manner and thus share similar network properties. In the analysis of high-dimensional data, clustering algorithm is often performed to reduce the dimensionality of the data. Variates in the same cluster exhibit similar patterns.

This may result in restrictions on the graphical gaussian models: equality among sepcified elements of the concentration matrix or equality emong specific partial variances and correlations. Adding symmetry to the graphical model reduces the number of parameters. When both sparsity and symmetry exisits, the likelihood estimation becomes computationally challenging.

Hojsgaard and Lauritzen (2009) introduced new types of Guassian models with symmetry constraints. When the restriction is imposed on the inverse convariance matrix, the model is referred as RCON model. When the restriction is imposed on the partial correlation matrix, the model is referred as RCOR model. Likelihood estimation on both models can be obtained through Newton iteration or partial maximization. However, the algorithm involves the inversion of concentration matrix in the interation steps, which can be computationally costly in the analysis of large matrices. When sparsity constrainst is imposed on the RCON and RCOR model, the likelihood is added extra penalty terms on the sizes of the edges. Solving the penalized likelihood with both sparsity and symmetry constraint is a challenge. In this article, we investigate the alternative way of formulating the likelihood. We propose to use composite likelihood as our objective function and maximize the penalized composite likelihood to obtain the sparse RCON and RCOR model. The algorithm is designed based on co-ordinate descent and soft thresholding rules. The algorithm is computationally convenient and it avoids any operations of large matrix inverison.

The rest of the article is organized as follows. In Section 2.1 we formulate the penalized likelihood function for the RCON and RCOR modle matrix. In Sections 2.2 and 2.3, we present the coordinate descent algorithm and soft thresholding rule. In Section 3, we investigate the asymptotic behavior of the estimate and establish the ORACLE property of the estimate. In Section 4, simulation studies are presented to demonstrate the empirical performance of the estimate in terms of estimation and model selection. In Section 5, we applied our method to a clustered microarray data set to estimate the networks between the clustered genes and also compare the networks under different treatment settings.

2. Method

2.1 Composite likelihood

The estimation of Gaussian graphical model has been mainly based on likelihood method. An alternative method of estimation based on composite likelihood has drawn much attention in recent years. It has been demonstrated to possess good theoretical properties, such as consistency for the parameter estimation, and can be utilized to establish hypothesis testing procedures. Let $x = (x_1, \ldots, x_n)^T$ be the vector of n variables observed from a single observation. Let $\{f(x; \phi), x \in \mathcal{X}, \phi \in \Psi\}$ be a class of parametric models, with $\mathcal{X} \subseteq \mathcal{R}^n$, $\Psi \subseteq \mathcal{R}^q$, $n \geq 1$, and $q \geq 1$. For a subset of $\{1, \ldots, n\}$, say a, x_a denotes a subvector of x with components indexed by the elements in set a; for instance, given a set $a = \{1, 2\}$, $x_a = (x_1, x_2)^T$. Let $\phi = (\theta, \eta)$, where $\theta \in \Theta \subseteq \mathcal{R}^p$, $p \leq q$, is the parameter of interest, and η is the nuisance parameter. According to Lindsay (1988), the CL of a single vector-valued observation is $L_c(\theta; x) = \prod_{a \in A} L_a(\theta; x_a)^{w_a}$, where A is a collection of index subsets called the composite sets, $L_a(\theta; x_a) = f_a(x_a; \theta_a)$, and $\{w_a, a \in A\}$ is a set of positive weights. Here f_a denotes all the different marginal densities and θ_a indicates the parameters that are identifiable in the marginal density f_a.

As the composite score function is a linear combination of several valid likelihood score functions, it is unbiased under the usual regularity conditions. Therefore, even though the composite likelihood is not a real likelihood, the maximum composite likelihood estimate is still consistent for the true parameter. The asymptotic covariance matrix of the maximum composite likelihood estimator takes the form of the inverse of the Godambe information:$H(\theta)^T J(\theta)^{-1} H(\theta)$, where $H(\theta) = E\{-\sum_{a \in A} \partial^2 \log f(x_a; \theta)/\partial\theta\partial\theta^T\}$ and $J(\theta) = \mathrm{var}\{\sum_{a \in A} \partial \log f(x_a; \theta)/\partial\theta\}$ are the sensitivity matrix and the variability matrix, respectively. Readers are referred to Cox and Reid (2004) and Varin (2008) for a more detailed discussion on the asymptotic behavior of the maximum composite likelihood estimator.

2.1 Composite likelihood estimation of rcon model

Let data X consist of n replications of a multivariate random vector of size p: $X = (X_1, X_2, \ldots, X_n)^T$, with $X_i = (X_{i1}, X_{i2}, \ldots, X_{ip})^T$ following a $N_p(\mu, \Sigma)$ distribution. For simplicity of exposition, we assume throughout that $\mu = 0$. We let $\theta = \Sigma^{-1}$ denote the inverse covariance, also known as the concentration matrix with elements (θ_{ij}), $1 \leq i, j, \leq p$. The partial correlation between X_{ij} and X_{ik} given all other variables is then

$$\rho_{jk} = -\theta_{jk}/\sqrt{\theta_{jj}\theta_{kk}}.$$

It can be shown than $\theta_{jk} = 0$ if and only if X_{ij} and X_{ik} are conditionally independent given all other variables.

There are different symmetry restrictions on cencentrations first introduced by Hojsgaard and Lauritzen (2009). An $RCON(\mathcal{V}, \mathcal{E})$ model with vertex coloring $\mathcal{V}$ and edge coloring $\mathcal{E}$ is obtained by restricting the elements of the concentration matrix θ as follows: 1) Diagonal elements of the concentration matrix θ corresponding to vertices in the same vertex colour class must be identical. 2) Off diagonal entries of θ corresponding to edges in the same edge colour class must be identical. Let $\mathcal{V} = \{V_1, \ldots, V_k\}$, where $V_1, \ldots, V_k$ is a partition of $\{1, \ldots, p\}$ vertex class. Let $\mathcal{E} = \{E_1, \ldots, E_l\}$, where $E_1, \ldots, E_l$ is a partition of $\{(i,j), 1 \leq i < j \leq p\}$ edge class. This implies given an edge color class, for all edges $(i,j) \in E_s$, θ_{ij} are all equal and hence denoted as θ_{E_s}. This also implies given a vertex color class, for all vertices $(i) \in V_m$, θ_{ii} are all equal and hence denoted as θ_{V_m}, σ^{ii} are all equal and hence denoted as σ_{V_m},

Following the approach of Friedman, Hastie and Tibshirani (2012), we formulate composite conditional likelihood to estimate sparse graphical model under symmetry constraints. The conditional distribution of $x_{ij}|x_{-ij} = N(\sum_{k\neq j} x_{ik}\beta_{kj}, \sigma^{jj})$, where $x_{-ij} = (x_{i1}, x_{i2}, \ldots, x_{i,j-1}, x_{j+1}, \ldots, x_{ip})$, $\beta_{kj} = -\theta_{kj}/\theta_{jj}$, and $\sigma^{jj} = 1/\theta_{jj}$. The negative composite log-likelihood can be formulated as

$$\ell_c(\theta) = \frac{1}{2}\sum_{j=1}^{p}(N\log\sigma^{jj} + \frac{1}{\sigma^{jj}}||X_j - XB_j||_2^2),$$

where B_j is a $p-$vector with elements β_{ij}, except a zero at the jth position, and $B = (B_1, B_2, \ldots, B_p)$. We propose to estimate the sparse RCON model by minimizing the following penalized composite loglikelihood $Q(\theta)$:

$$\min_{\theta_{E_s},1\leq s\leq l,\theta_{V_m},1\leq m\leq k} \ell_c(\theta) + n\lambda\sum_s|\theta_{E_s}|.$$

We employ coordinate-descent algorithm by solving the penalized minimization one coordinate at a time. It can be shown that the negative expected Hessian matrix of $\ell_c(\theta)$ is positive definite because it is the sum of expected negative Hessian matrices of all conditional likelihoods:

$$\begin{aligned}&E(\frac{-\partial^2\ell_c(\theta)}{\partial\theta^2}) = \sum_{i=1}^{n}\sum_{j=1}^{p}E(\frac{\partial^2 l(x_{ij}|x_{-ij})}{\partial\theta^2})\\ =&\sum_{i=1}^{n}\sum_{j=1}^{p}E(E(\frac{\partial^2 l(x_{ij}|x_{-ij})}{\partial\theta^2}|x_{-ij})) = \sum_{i=1}^{n}\sum_{j=1}^{p}E(\text{var}(\frac{\partial l(x_{ij}|x_{-ij})}{\partial\theta}|x_{-ij})).\end{aligned} \tag{1}$$

Each $\text{var}(\frac{\partial l(x_j|x_{-j})}{\partial\theta}|x_{-j})$ is positive definite and integrals preserve positive definiteness, therefore $E(\frac{\partial^2\ell_c(\theta)}{\partial\theta^2})$ is positive definite. Thus, when n is sufficiently larege, the objective function $Q(\theta)$ is locally convex at θ_0. If the interation steps of the algorithm hits this neighborhood, the algorithm will converge to θ_0.

The co-ordinate descent algorithm proceeds by updating each parameter of the objective function one at a time. The first derivative of the objective function with respect to the edge class parameter is as follows. The technical derivation is in the Appendix.

$$\begin{aligned}\frac{\partial Q(\theta)}{\partial\theta_{E_s}} =&(\sum_{j=1}^{p}\sum_{i;(i,j)\in E_s}\sum_{l;(l,j)\in E_s}\sigma^{jj}X_i^T X_l)\theta_{E_s}+\\ &\left(\sum_{j=1}^{p}X_j^T(\sum_{i;(i,j)\in E_s}X_i) + \sigma^{jj}\sum_{i;(i,j)\in E_s}\sum_{l;(l,j)\in E_s^c}X_i^T X_l\theta_{lj}\right) + n\text{sgn}(\theta_{E_s}),\end{aligned} \tag{2}$$

where $E_s^c = \{(i,j)|i \neq j \text{ and } (i,j) \notin E_s\}$. Therefore the update for θ_{E_s} is

$$\hat{\theta}_{E_s} = \frac{S(-(\sum_{j=1}^p X_j^T(\sum_{i;(i,j)\in E_s} X_i) + \sigma^{jj}\sum_{i;(i,j)\in E_s}\sum_{l;(l,j)\in E_s^c} X_i^T X_l \theta_{lj})/n, \lambda)}{(\sum_{j=1}^p \sum_{i;(i,j)\in E_s}\sum_{l;(l,j)\in E_s} \sigma^{jj} X_i^T X_l)/n},$$

where $S(z,\lambda) = \text{sign}(z)(|z|-\lambda)_+$ is the soft-thresholding operator. Let $C = \frac{1}{n}X^T X$ denote the sample covariance matrix. Given the color edge group E_s, we construct the edge adjancency matrix T^{E_s}, with $T_{ij}^{E_s} = 1$, if $(i,j) \in E_s$, and $T_{ij}^{E_s} = 0$ otherwise. We can simplify the updating expression as follows:

$$\hat{\theta}_{E_s} = \frac{S(-\text{tr}(T^{E_s}C) + \text{tr}(T^{E_s}(T^{E_s^c} \odot B)C), \lambda)}{\text{tr}(T^{E_s}(T^{E_s}\sigma)C)},$$

where $\odot$ denotes the componentwise product, and σ denotes a $p \times p$ matrix of $\text{diag}(\sigma^{jj})$.

For notational convenience, let $\tilde{\theta}$ denote a $p \times p$ matrix with diagonal elements equal to zero and off-diagonal elements equal to that of θ. The first derivative of $Q(\theta)$ with respect to the vertex class is as follows:

$$\begin{aligned} &\frac{\partial Q(\theta)}{\partial \sigma_{V_m}} \\ =&\frac{n}{2}\sum_{j\in V_m}\left(\frac{1}{\sigma^{jj}} - \frac{C_{jj}}{(\sigma^{jj})^2} + q_j\right), \end{aligned} \tag{3}$$

where $q_j = \sum_{l=1}^p \sum_{l'=1}^p C_{ll'}\tilde{\theta}_{lj}\tilde{\theta}_{l'j}$. Therefore the solution of

$$\hat{\sigma}_{V_m} = \frac{-|V_m| + \sqrt{|V_m|^2 + 4(\sum_{j\in V_m} q_j)(\sum_{j\in V_m} C_{jj})}}{2\sum_{j\in V_m} q_j},$$

where $|V_m|$ denotes the cardinality of V_m. Let diagonal matrix T^{V_m} denote the generator for the vertex color class, with $T_{jj}^{V_m} = 1$ for $j \in V_m$, and $T_{jj}^{V_m} = 0$ otherwise. To simplify the notation, we have $\sum_{j\in V_m} C_{jj} = \text{tr}(T^{V_m}C)$, and $\sum_{j\in V_m} q_j = \text{tr}(T^{V_m}\tilde{\theta}C\tilde{\theta})$. Because C is positive definite, $\sum_{j\in V_m} q_j > 0$. Therefore, the quadratic equation has one unique positive root. Alternating the updating scheme throughout all the θ_{E_s}, and θ_{V_m} until convergence, we obtain the penalized sparse estimate of the concentration matrix under RCON model.

2.2 Estimation of rcor model

An RCOR $(\mathcal{V}, \mathcal{E})$ model with vertex colouring $\mathcal{V}$ and edge coloring $\mathcal{E}$ is obtained by restricting the elements of θ as follows: (a) All diagonal elements of θ (inverse partial variances) corresponding to vertices in the same vertex colour class must be identical. (b) All partial correlations corresponding to edges in the same edge colour class must be identical. Given an edge color class, for all edges $(i, j) \in E_s$, ρ_{ij} are all equal and hence denoted as ρ_{E_s}. This also implies given a vertex color class, for all vertices $(i) \in V_m$, θ_{ii} are all equal and hence denoted as θ_{V_m}, and σ^{ii} are all equal and hence denoted as σ_{V_m}, We formulate the composite likelihood in terms of ρ_{E_s} and σ_{V_m}.

For notational convenience, define a $p \times p$ matrix $\tilde{\rho}$ with $\tilde{\rho}_{ij} = \rho_{ij}$ for $i \neq j$ and $\tilde{\rho}_{ij} = 0$ for $i = j$. Let $\tilde{\rho}_j$ denote the jth column of the matrix $\tilde{\rho}$. Define a p-element vector $\sigma_D = (\sigma^{11}, \ldots, \sigma^{pp})^T$. The composite likelihood is formulated as

$$\ell_c(\rho, \sigma) = \frac{1}{2} \sum_{j=1}^{p} \{n \log \sigma^{jj} + \frac{1}{\sigma^{jj}} ||X_j - X(\tilde{\rho}_j \odot \sigma_D^{-\frac{1}{2}})(\sigma^{jj})^{\frac{1}{2}}||_2^2\}.$$

We propose to estimate the sparse RCOR model by minimizing the following penalized composite loglikelihood $Q(\rho, \sigma)$:

$$\min_{\theta_{E_s}, 1 \leq s \leq l, \theta_{V_m}, 1 \leq m \leq k} \ell_c(\rho, \sigma) + n\lambda \sum_{s} |\rho_{E_s}|.$$

The partial derivative of $Q(\rho, \sigma)$ with respect to the partial correlation is as follows:

$$\begin{aligned} &\frac{\partial Q(\rho, \sigma)}{\partial \rho_{E_s}} \\ =& n\rho_{E_s} \mathrm{tr}\Big((\sigma^{-1/2} T^{E_s})^T C (\sigma^{-1/2} T^{E_s}) \Big) + n \mathrm{tr}\Big((\sigma^{-1/2} \tilde{\rho} \odot T^{E_s^c})^T C (\sigma^{-1/2} T^{E_s}) \Big) \\ &- \mathrm{tr}\Big((X\sigma^{-1/2})^T X (\sigma^{-1/2} T^{E_s}) \Big) + n \mathrm{sgn}(\theta_{E_s}). \end{aligned} \tag{4}$$

The thresholded estimate of the partial correlation takes the following form:

$$\tilde{\rho}_{E_s} = \frac{S(\mathrm{tr}(T^{E_s}(\sigma^{-\frac{1}{2}} C \sigma^{-\frac{1}{2}})) - \mathrm{tr}(T^{E_s}(T^{E_s^c} \odot \tilde{\rho})(\sigma^{-\frac{1}{2}} C \sigma^{-\frac{1}{2}})), \lambda)}{\mathrm{tr}(T^{E_s}.T^{E_s}(\sigma^{-\frac{1}{2}} C \sigma^{-\frac{1}{2}}))}.$$

The partial derivatives with respect to σ_{V_m} is as follows:

$$
\begin{aligned}
&\frac{\partial \ell(\rho,\sigma)}{\partial \sigma_{V_m}}\\
=&\frac{n}{2}\{\frac{|V_m|}{\sigma_{V_m}} - \frac{\sum_{j\in V_m} x_j^T x_j}{n\sigma_{V_m}^2} + \frac{\sum_{i\in V_m}\sum_{j\in V_m} 2x_i^T x_j \tilde{\rho}_{ij}}{n\sigma_{V_m}^2} + \frac{2}{n}\sigma_{V_m}^{-\frac{3}{2}} \sum_{(i,j);i\in V_m, j\notin V_m} x_i^T x_j \tilde{\rho}_{ij}/\sqrt{\sigma_{jj}}\\
&-\frac{1}{n\sigma_{V_m}^2}\sum_{j=1}^{p}\sum_{i\in V_m}\sum_{i'\in V_m} x_i^T x_{i'} \tilde{\rho}_{ij}\tilde{\rho}_{i'j} - \frac{1}{n\sigma_{V_m}^{\frac{3}{2}}}\sum_{j=1}^{p}\sum_{i\in V_m}\sum_{i'\notin V_m} x_i^T x_{i'}\tilde{\rho}_{ij}\tilde{\rho}_{i'j}/\sqrt{\sigma^{i'i'}}\}.
\end{aligned} \tag{5}
$$

Re-express the above expression in terms of $y = \sqrt{\sigma_{V_m}}$. We solve the equation

$$|V_m|y^2 - by - a = 0,$$

with

$$
\begin{aligned}
a &= \sum_{j\in V_m} x_j^T x_j/n - \sum_{i\in V_m}\sum_{j\in V_m} 2x_j^T x_i \tilde{\rho}_{ij}/n + \sum_{j=1}^{p}\sum_{i\in V_m}\sum_{i'\in V_m} x_i^T x_{i'}\tilde{\rho}_{ij}\tilde{\rho}_{i'j}/n\\
&= \mathrm{tr}(T^{V_m}C) - 2\mathrm{tr}(T^{V_m}CT^{V_m}\tilde{\rho})) + \mathrm{tr}(\tilde{\rho}T^{V_m}CT^{V_m}\tilde{\rho})
\end{aligned} \tag{6}
$$

and

$$
\begin{aligned}
b &= -\sum_{i\in V_m}\sum_{j\notin V_m} 2x_j^T x_i\tilde{\rho}_{ij}/(n\sqrt{\sigma^{jj}}) + \sum_{j=1}^{p}\sum_{i\in V_m}\sum_{i'\notin V_m} x_i^T x_{i'}\tilde{\rho}_{ij}\tilde{\rho}_{i'j}/(n\sqrt{\sigma^{i'i'}})\\
&= -2\mathrm{tr}(T^{V_m}C\sigma^{-1/2}T^{V_m^c}\tilde{\rho}) + \mathrm{tr}(\tilde{\rho}T^{v_m^c}\sigma^{-1/2}CT^{V_m}\tilde{\rho}).
\end{aligned} \tag{7}
$$

The solution would be

$$y = \frac{b + \sqrt{b^2 + 4a|V_m|}}{2|V_m|}.$$

The positive solution is unique because

$$a = \mathrm{tr}\Bigg(C(T^{V_m} - \tilde{\rho}T^{V_m})^T(T^{V_m} - \tilde{\rho}T^{V_m})\Bigg) > 0. \tag{8}$$

2.3 Asymptotic properties

In this section, we discuss the asymptotic properties of the penalized composite likelihood estimates for sparse symmetric Gaussian graphical models. In terms of the choice of penalty function, there are many penalty functions available. As the LASSO penalty,

$p_\lambda(|\theta_l|) = \lambda|\theta_l|$, increases linearly with the size of its argument, it leads to biases for the estimates of nonzero coefficients. To attenuate such estimation biases, Fan and Li (2001) proposed the SCAD penalty. The penalty function satisfies $p_\lambda(0) = 0$, and its first-order derivative is

$$p'_\lambda(\theta) = \lambda\{I(\theta \leq \lambda) + \frac{(a\lambda - \theta)_+}{(a-1)\lambda} I(\theta > \lambda)\}, \text{ for } \theta \geq 0,$$

where a is some constant, usually set to 3.7 (Fan and Li, 2001), and $(t)_+ = tI(t > 0)$ is the hinge loss function. The SCAD penalty function does not penalize as heavily as the L_1 penalty function on parameters with large values. It has been shown that with probabability tending to one, the likelihood estimation with the SCAD penalty not only selects the correct set of significant covariates, but also produces parameter estimators as efficient as if we know the true underlying sub-model (Fan & Li, 2001). Namely, the estimators have the so-called ORACLE property. However, it has not been investigated if the oracle property is also enjoyed by composite likelihood estimation of GGM with the SCAD penalty. The following discussion is focused on the RCON model but it can be easily extended to RCOR model.

For notational convenience, let $z = \{E_s : \theta_{E_s} \neq 0\} \cup \mathcal{V}$ denote all the nonzero edge classes and all vertex classes and $z^c = \{E_s : \theta_{E_s} = 0\}$ denote all the zero edge classes. The parameter vector can be expressed as $\theta = (\theta_{E_1}, \ldots, \theta_{E_l}, \theta_{V_1}, \ldots, \theta_{V_k})$. Let θ_0 denote the true null value.

Theorem 1. *Given the SCAD penalty function $p_\lambda(\theta)$, if $\lambda_n \to 0$, and $\sqrt{n}\lambda_n \to \infty$ as $n \to \infty$, then there exist a local maximizer $\hat{\theta}$ to $Q(\theta)$ and $||\hat{\theta} - \theta_0|| = O_p(n^{\frac{1}{2}})$. Furthermore, we have*

$$\lim_{n\to\infty} P(\hat{\theta}_{z^c} = 0) = 1.$$

Proof. Consider a ball $||\theta - \theta_0|| \leq Mn^{-\frac{1}{2}}$ for some finite M. Applying Taylor Expansion, we obtain:

$$\begin{aligned}\partial Q(\theta)/\partial\theta_j &= \partial\ell_c(\theta)/\partial\theta_j - np'_{\lambda_n}(|\theta_j|)\text{sign}(\theta_j)\\ &= \partial\ell_c(\theta_0)/\partial\theta_j + \sum_{j'\in(\mathcal{E}\cup\mathcal{V})}(\theta_{j'}-\theta_{j'0})\partial^2\ell_c(\theta^*)/\partial\theta_j\theta_{j'} - np'_{\lambda_n}(|\theta_j|)\text{sign}(\theta_j),\end{aligned} \tag{9}$$

for $j \in (\mathcal{E}\cup\mathcal{V})$ and some θ^* between θ and θ_0. As $E(\partial\ell_c(\theta_0)/\partial\theta_j) = 0$, $\partial\ell_c(\theta_0)/\partial\theta_j = O_p(n^{\frac{1}{2}})$. As $|\theta^*-\theta| \le Mn^{-\frac{1}{2}}$ and $\partial^2\ell_c(\theta^*)/\partial\theta_j\theta_{j'} = O_p(n)$ componentwise. First we consider $j \in z^c$. Because lim $\inf_{n\to\infty}$lim $\inf_{\beta\to 0+}p'_{\lambda_n}(\beta)/\lambda_n > 0$, and $\lambda_n \to 0$, and $\sqrt{n}\lambda_n \to \infty$ as $n \to \infty$, the third term dominates the the first two terms. Thus the sign of $\partial Q(\theta)/\partial\theta_j$ is completely determined by the sign of β_j. This entails that inside this $Mn^{-1/2}$ neighborhood of β_0, $\partial Q(\theta)/\partial\theta_j > 0$, when $\theta_j < 0$ and $\partial Q(\theta)/\partial\theta_j < 0$, when $\theta_j > 0$. Therefore for any local maximizer $\hat\theta$ inside this ball, then $\hat\theta_j = 0$ with probability tending to one. As $p_{\lambda_n}(0) = 0$, we obtain

$$\begin{aligned}Q(\theta)-Q(\theta_0) &= \ell_c(\theta)-\ell_c(\theta_0) - n\sum_{j\in(\mathcal{E}\cup\mathcal{V})}\big(p_{\lambda_n}(|\theta_j|)-p_{\lambda_n}(|\theta_{j0}|)\big)\\ &\le (\theta-\theta_0)^T\frac{\partial\ell_c(\theta_0)}{\partial\theta} + (\theta-\theta_0)^T\frac{\partial^2\ell_c(\theta^*)}{\partial\theta^2}(\theta-\theta_0)\\ &\quad - n\sum_{j\in z}\Big(p'_{\lambda_n}(|\theta_{j0}|)\text{sign}(\theta_{j0})(\theta_j-\theta_{j0}) + p''_{\lambda_n}(|\theta_{j0}|)(\theta_j-\theta_{j0})^2(1+o(1))\Big).\end{aligned} \tag{10}$$

For n large enough and $\theta_{j0}\neq 0$, $p'_\lambda(|\theta_{j0}|) = 0$ and $p''_\lambda(|\theta_{j0}|) = 0$. Furthermore, $\partial^2\ell_c(\theta^*)/\partial\theta^2$ converges to $H(\theta)$ in probability, which is negative definite. Thus, we have $Q(\theta)\le Q(\theta_0)$ with probability tending to one for θ on the unit ball. This implies there exists a local maximizer of $\hat\theta$ such that $|\hat\theta-\theta_0| = O_p(n^{-1/2})$. □

Next, we establish the asymptotic distribution of the estimator $\hat\theta$. Let θ_z denote the sub-vector of nonzero parameters in θ. Define a matrix $\Sigma_1 = \text{diag}\{p''_{|\lambda_n|}(\theta_{j0}); j\in z\}$, and a vector $b_1 = (p'_{\lambda_n}(\theta_j)\text{sign}(\theta_{j0}); j\in z)$. Let H_{zz} denote the sub-matrix of $H(\theta)$ and V_{zz} denote the sub-matrix of $V(\theta)$ corresponding to the subset of z.

Theorem 2. *Given the SCAD penalty function $p_\lambda(\theta)$, if $\lambda_n \to 0$ and $\sqrt{n}\lambda_n \to \infty$, as $n \to \infty$, then the sub-vector of the root-n consistent estimator $\hat{\theta}_z$ has the following asymptotic distribution:*

$$\sqrt{n}(H_{zz} + \Sigma_1)\{\hat{\theta}_z - \theta_{z0} + (H_{zz} + \Sigma_1)^{-1} b_1\} \to N\{0, V_{zz}\},\ as\, n \to \infty.$$

Proof. Based on Taylor expansion presented in Proof to Theorem 1, we have

$$0 = \frac{\partial Q(\hat{\theta})}{\partial \theta_z} = \frac{\partial \ell_c(\theta_0)}{\partial \theta_z} + \frac{\partial^2 \ell_c(\theta^*)}{\partial \theta_z \partial \theta_z^T}(\hat{\theta}_z - \theta_{z0}) - nb_1 - n(\Sigma_1 + o(1))(\hat{\theta}_z - \theta_{z0}). \quad (11)$$

As $\hat{\theta} \to \theta_0$ in probability, $\frac{1}{n}\frac{-\partial^2 \ell_c(\theta^*)}{\partial \theta_z \partial \theta_z^T} \to H_{zz}$ in probability. The limiting distribution of $\frac{1}{\sqrt{n}}\frac{\partial \ell_c(\theta_0)}{\partial \theta_z}$ is $N\{0, V_{zz}\}$. According to Slutsky's theorem, we have$\sqrt{n}(H_{zz} + \Sigma_1)\{\hat{\theta_z} - \theta_{z0} + (H_{zz} + \Sigma_1)^{-1} b_1\} \to N\{0, V_{zz})\}$. □

Next we discuss the estimation of the Hessian matrix H_{zz} and the variability matrix V_{zz}. As the second differentiation is easy to calculate, we obtain $\hat{H}_{zz} = \partial^2 \ell_c(\theta)/\partial \theta_z \partial \theta_z^T|_{\hat{\theta}}$. The variability matrix based on sample covariance matrix of the composite score vectors is computationally harder as we need to compute the composite score vector for each observation, where the number of observations can be large. Alternatively, we perform bootstrap to obtain the

$$\hat{V}_{zz} = \frac{1}{n(m-1)} \sum_{l=1}^{m} (S^{(m)}(\hat{\theta}) - \overline{S})^T (S^{(m)}(\hat{\theta}) - \overline{S}),$$

where $S(\theta) = \partial \ell_c(\theta)/\partial \theta_z$, $S^{(m)}(\hat{\theta})$ denotes the score vector evaluated with the composite estimator obtained from the original sample and the data from the mth bootstrap sample and $\overline{S} = \sum_{l=1}^{m} S^{(m)}(\hat{\theta})/m$. In pratice, we only need a moderate number of bootstrap samples to obtain $\hat{V}_{zz}$.

3. Numerical analysis

We analyze the "math" data set from Mardia et al. (1979), which consists of 88 students in 5 different mathematics subjects: Mechanics (me), Vectors (ve), Algebra (al), Analysis (an) and Statistics (st). The model with symmetry proposed by Hojsgaard and Lauritzen (2008) has vertex color classes {al}, {me, st}, {ve, an} and edge color classes {(al,an)}, {(an,st)}, {(me,ve), (me,al)}, and {(ve,al), (al,st)}. We perform composite likelihood estimation on this symmetric model with no penalty imposed on the parameters. In Table 1, the composite likelihood estimates and their standard deviations calculated through bootstraps are compared with those obtained by maximum likelihood estimator and a naive estimator. The naive estimator estimates the edge class parameters and vertex class parameters by simply averaging all the values belonging to the same class in the inverse sample covariance matrix. All three methods yield results that are very close to each other.

Next we examine the performance of the unpenalized composite likelihood estimator on large matrices. First we consider the RCON model. We simulate under different scenarios with n varying from 250 to 1000 and p varying from 40, 60 to 100. We include 30 different edge classes and 20 different vertex classes. We simulate a sparse matrix with $\theta_{\mathcal{E}} = (0_{25}, 0.2591, 0.1628, -0.1934, 0.0980, 0.0518)$, and $\theta_{\mathcal{V}} = (1.3180, 1.8676, 1.788004, 1.7626, 1.6550, 1.1538, 1.3975, 1.7877, 1.7090, 1.6931, 1.46313, 1.5131, 1.7084, 1.7344, 1.1441, 1.8059, 1.7446, 1.8522, 1.3146, 1.1001)$, where 0_p denotes a zero vector of length p. The number of nonzero edges ranges from about 250 to 1640. In Table 2, we compare the sum of squared errors of the composite likelihood estimates with the naive estimates from 100 simulated data sets. The proposed composite likelihood estimates consistenly enjoy much smaller sum of squared errors across all settings.

We also investigate the empirical performance of the proposed composite likelihood estimator under the RCOR model. We simulate under different scenarios with n varying from 250 to 1000 and p varying from 40, 60 to 100. We include 30 different edge classes and 20 different vertex classes. We simulate a sparse matrix with $\rho_{\mathcal{E}} = (0_{26}, 0.1628, -0.1534, 0.0980, 0.0518)$ and $\theta_{\mathcal{V}} = (3.0740, 3.6966, 3.7772, 3.5475, 3.2841, 3.4699, 3.7235, 3.5987,$

$3.3313, 3.8183, 3.9236, 3.9008, 3.9011, 3.0470, 3.0139, 3.2072, 3.8438, 3.4823, 3.9373, 3.0125.$)
In table 3, we provide the errors $||\hat{\rho}_{\mathcal{E}} - \rho_{\mathcal{E}}||_2$ and $||\sqrt{\hat{\sigma}}_{\mathcal{V}} - \sqrt{\hat{\sigma}}_{\mathcal{V}}||_2$ for the composite likelihood estimates and the naive estimates from 100 simulated data sets. With regard to the estimated partial correlations, the composite likelihood estimates yield consistently smaller errors compared to the naive estimates. With regard to the conditional standard deviations, the composite likelihood estimates yield slightly larger errors under sample size $n = 250$, and $n = 500$. With sample size $n = 1000$, the composite likelihood estimates have smaller errors than the naive estimates. For example, with $p = 100$ and the number of true edges close to 1300, the naive estimate for the conditional standard deviation has error 1.8116, while the composite likelihood estimate has error 0.2923.

We further examine the empirical performance of the penalized composite likelihood estimator. We simulate the RCON model using the same settings as of Table 1. We consider different scenarios with $n = 250$ or $n = 500$, and $p = 40$ or $p = 60$. We use the penalized composite likelihood estimator to estimate the sparse matrix. The tuning parameter is selected by composite BIC, which is similar to BIC with the first term replaced by the composite likelihood evaluated at the penalized composite likelihood estimates. For each setting, 100 simulated data sets are generated and for each data we calculate the number of false negatives and false positives. In Table 4, it is shown that the proposed method has satisfactory model selection property with very low false negative and false positive results. For example, with $n = 500$ and $p = 60$, each simulated data set has an average number of 1474 zero edges and 325 nonzero edges. The proposed method identifies an average of zero false negative result and 0.58 false positive result. The size of the tuning parameters is also listed in Table 4.

5. Applicattion

We apply the proposed method on a real biological data set. The experiment was conducted to examine how GM-CSF modulates global changes in neutrophil gene expressions (Kobayashi et al, 2005). Time course summary PMNs were isolated from venous blood of healthy individuals. Human PMNs (107) were cultured with and without 100 ng/ml GM-CSF for up to 24 h. The Experiment was performed in triplicate, using PMNs from three healthy individuals for each treatment. There are in total 12625 genes monitored, each gene is measured for 9 replications at time 0, and measured for 6 times at time 3, 6, 12, 18, 24h. At each of these 5 points, 3 measurements were obtained for treatment group and 3 measurements were obtained for control group. We first proceed with standard gene expression analysis. For each gene, we perform an ANOVA test on the treatment effect while aknowledging the time effet. We rank the F statistic for each gene and select the top 200 genes who have the most significant changes in expression between treatment and control group. Our goal is to study the networks of these 200 genes and also compare the network of the 200 genes between the treatment and control. We perform clustering analysis on the selected 200 genes, where the genes clustered together can be viewed as a group of genes who share similar expression profiles. This imposes symmetry constraints to the graphical modelling. We cluster these top 200 genes into 10 clusters based on K-means method. Therefore, there are in total of 55 edge classes and 10 vertex classes to be estimated based on a 200 by 200 data matrices. We perform penalized estimation and compare the result of the estimated edges between the treatment versus control. The estimated between-cluster edges are provided in Figure 1. It is observed that although most between-cluster interactions are small, there are a few edges with large values indicating strong interactions. It is also observed that the edge values obtained from the treatment group and the control group are mostly comparable and only a few edges exhibit big differences. For instance, edges between cluster 1 and 5 and between cluster 4 and 6 have big differences in treatment group versus control group. These findings are worth further biological investigation to unveil the physical mechanism underlying the networks.

6. Conclusion

When there are both sparsity and symmetry constrainsts on the graphical model, the penalized composite likelihood formulation based on conditional distributions offers an alternative way to perform the estimation and model selection. The estimation avoids the inversion of large matrices. It is shown that the proposed penalized composite likelihood estimator will threshold the estimate for zero parameters to zero with probability tending to one and the asymptotic distribution of the estimates for non-zero parameters follow the multivariate normal distribution as if we know the true submodel containing only non-zero parameters.

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Appendix

- The detailed derivation of the first derivatives with respect to θ_{E_s} under RCON model is as follows:

$$
\begin{aligned}
&\frac{\partial Q(\theta)}{\partial \theta_{E_s}} \\
=&\sum_{j=1}^{p} \frac{1}{2\sigma^{jj}} \frac{\partial ||X_j + X\tilde{\theta}_j\sigma^{jj}||_2^2}{\partial \theta_{E_s}} + n\text{sgn}(\theta_{E_s}) \\
=&\sum_{j=1}^{p} \frac{1}{\sigma^{jj}} (X_j + X\tilde{\theta}_j\sigma^{jj})^T \frac{\partial (X_j + X\tilde{\theta}_j\sigma^{jj})}{\partial \theta_{E_s}} + n\text{sgn}(\theta_{E_s}) \\
=&\sum_{j=1}^{p} (X_j + X\tilde{\theta}_j\sigma^{jj})^T (\sum_{i;(i,j)\in E_s} X_i) + n\text{sgn}(\theta_{E_s}) \\
=&\sum_{j=1}^{p} (X_j^T (\sum_{i;(i,j)\in E_s} X_i) + \sigma^{jj} (\sum_{i;(i,j)\in E_s} X_i^T (\sum_{l;(l,j)\in E_s} X_l\theta_{E_s} + \sum_{l;(l,j)\notin E_s} X_l\theta_{lj}))) + n\text{sgn}(\theta_{E_s}) \\
=&(\sum_{j=1}^{p} \sum_{i;(i,j)\in E_s} \sum_{l;(l,j)\in E_s} \sigma^{jj} X_i^T X_l)\theta_{E_s} + \Bigg(\sum_{j=1}^{p} X_j^T (\sum_{i;(i,j)\in E_s} X_i) + \\
&\sigma^{jj} \sum_{i;(i,j)\in E_s} \sum_{l;(l,j)\notin E_s} X_i^T X_l \theta_{lj}\Bigg) + n\text{sgn}(\theta_{E_s}).
\end{aligned} \tag{12}
$$

- The detailed derivation of the first derivatives with respect to θ_{V_m} under RCON model is as follows:

$$
\begin{aligned}
&\frac{\partial Q(\theta)}{\partial \sigma_{V_m}} \\
=&\frac{1}{2} \sum_{j\in V_m} \frac{n}{\sigma^{jj}} + \partial\{\frac{(X_j + X\tilde{\theta}_j\sigma^{jj})^T (X_j + X\tilde{\theta}_j\sigma^{jj})}{\sigma^{jj}}\}/\partial\sigma^{jj} \\
=&\frac{n}{2} \sum_{j\in V_m} (\frac{1}{\sigma^{jj}} - \frac{C_{jj}}{(\sigma^{jj})^2} + q_j),
\end{aligned} \tag{13}
$$

where $C_{ij} = x_i^T x_j/n$, and $q_j = \sum_{l=1}^{p} \sum_{l'=1}^{p} C_{ll'} \tilde{\theta}_{lj} \tilde{\theta}_{l'j}$.

- The detailed derivation of the first derivatives with respect to ρ_{E_s} under RCOR model is as follows:

$$\begin{aligned}&\frac{\partial Q(\rho,\sigma)}{\partial \rho_{E_s}}\\ =&\sum_{j=1}^{p}\frac{1}{\sqrt{\sigma^{jj}}}\bigg(X(\tilde{\rho}_j\odot\sigma_D^{-1/2})\sqrt{\sigma^{jj}}-X_j\bigg)^T X(\frac{\partial\tilde{\rho}_j}{\partial\rho_{E_s}}\odot\sigma_D^{-1/2})+n\text{sgn}(\theta_{E_s}).\end{aligned}\tag{14}$$

Note that $(\tilde{\rho}_j\odot\sigma_D^{-1/2})=(\sigma^{-1/2}\tilde{\rho})_{[,j]}$, the jth column of the matrix. Also we have the vector $\frac{\partial\tilde{\rho}_j}{\partial\rho_{E_s}}\odot\sigma_D^{-1/2}=(\sigma^{-1/2}T^{E_s})_{[,j]}$ the jth column of the matrix. Furthermore, $\tilde{\rho}=\sum_{s'}\rho_{E_{s'}}T^{E_{s'}}$. This leads to:

$$\begin{aligned}&\frac{\partial Q(\rho,\sigma)}{\partial \rho_{E_s}}\\ =&\sum_{j=1}^{p}\rho_{E_s}(\sigma^{-1/2}T^{E_s})_{[,j]}X^TX(\sigma^{-1/2}T^{E_s})_{[,j]}+(\sigma^{-1/2}\tilde{\rho}\odot T^{E_s^c})_{[,j]}X^TX(\sigma^{-1/2}T^{E_s})_{[,j]}\\ &-\frac{1}{\sqrt{\sigma^{jj}}}X_j^TX(\sigma^{-1/2}T^{E_s})_{[,j]}+n\text{sgn}(\theta_{E_s})\\ =&n\rho_{E_s}\text{tr}\bigg((\sigma^{-1/2}T^{E_s})^TC(\sigma^{-1/2}T^{E_s})\bigg)+n\text{tr}\bigg((\sigma^{-1/2}\tilde{\rho}\odot T^{E_s^c})^TC(\sigma^{-1/2}T^{E_s})\bigg)\\ &-\text{tr}\bigg((X\sigma^{-1/2})^TX(\sigma^{-1/2}T^{E_s})\bigg)+n\text{sgn}(\theta_{E_s}).\end{aligned}\tag{15}$$

Table 1: Comparison of likelihood, composite likelihood, moment estimates on "math" dataset

parameter	est	std	est	std	est	std
	likelihood		composite		moment	
vcc1	0.0281	0.0037	0.0068	0.0005	0.0057	0.0005
vcc2	0.0059	0.0006	0.0074	0.0006	0.0098	0.0013
vcc3	0.0100	0.0009	0.0176	0.0020	0.0182	0.0029
ecc1	-0.0080	0.0015	-0.0062	0.0009	-0.0068	0.0019
ecc2	-0.0018	0.0007	-0.0008	0.0005	-0.0021	0.0008
ecc3	-0.0030	0.0004	-0.0027	0.0002	-0.0019	0.0006
ecc4	-0.0047	0.0008	-0.0051	0.0005	-0.0055	0.0012

Table 2: Comparison of $||\theta - \hat{\theta}||_2^2$ from composite likelihood and moment estimates on simulated large dataset for RCON model

n	p	comp	moment	#true edges
250	40	0.2002	2.3671	256.7475
		(0.0757)	(0.4580)	(15.5644)
250	60	0.1109	5.6270	590.4040
		(0.0367)	(0.7201)	(23.5606)
250	100	0.0509	23.7040	1647.0707
		(0.0155)	(2.0364)	(34.7461)
500	40	0.0901	0.5482	256.7475
		(0.0272)	(0.1439)	(15.5644)
500	60	0.0588	1.0924	590.4040
		(0.0177)	(0.1728)	(23.5606)
500	100	0.0252	3.3530	1647.0707
		(0.0098)	(0.2781)	(34.7461)
1000	40	0.0467	0.1548	256.7475
		(0.0160)	(0.0444)	(15.5644)
1000	60	0.0282	0.2596	590.4040
		(0.0090)	(0.0491)	(23.5606)
1000	100	0.0125	0.6686	1647.0707
		(0.0037)	(0.0684)	(34.7461)

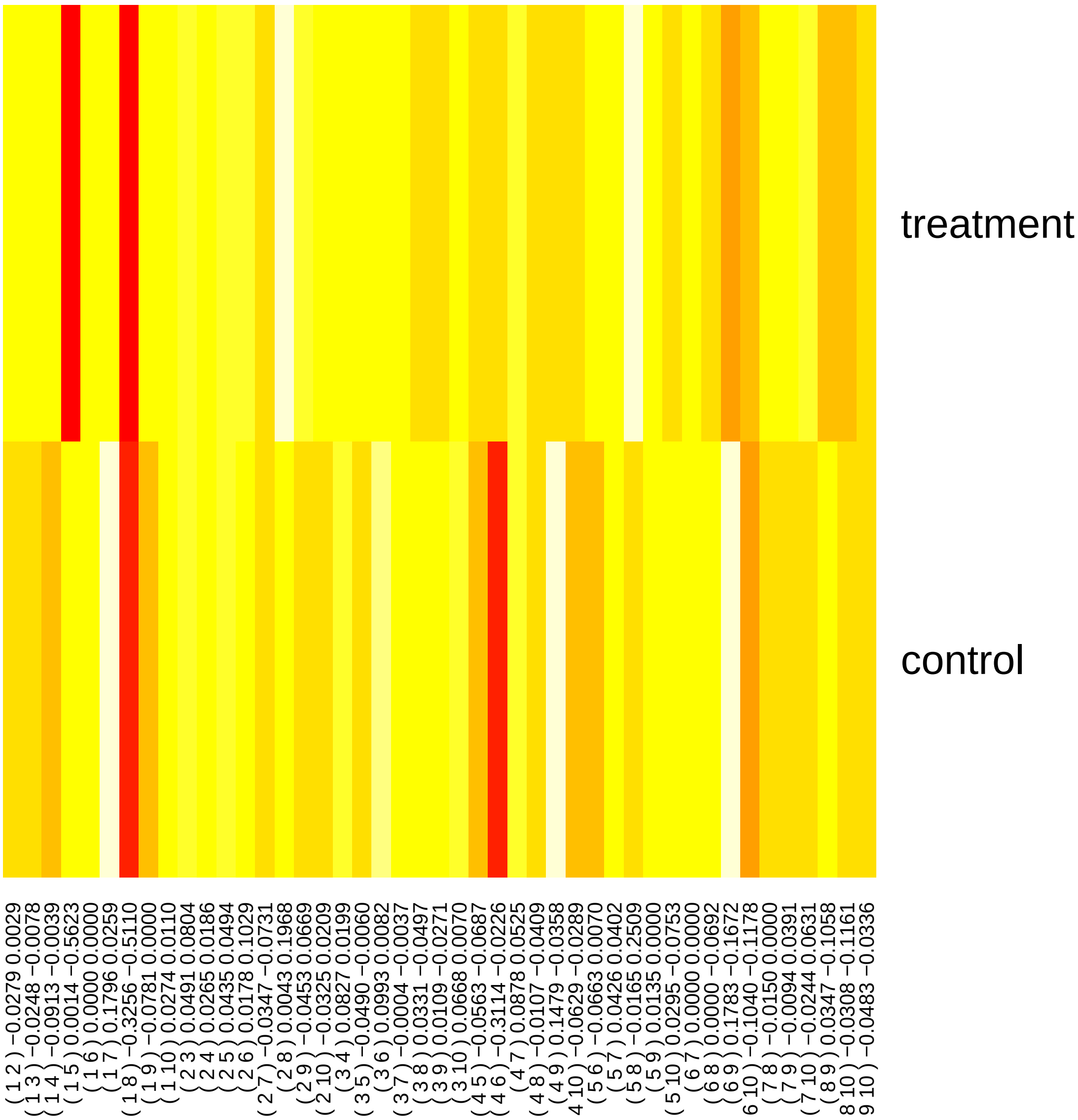
Table 3: Comparison of the composite likelihood and moment estimates on simulated large dataset for RCOR model

n	p	comp $\|\|\hat{\rho}-\rho_0)\|\|_2$	moment $\|\|\tilde{\rho}-\rho_0)\|\|_2$	comp $\|\|\hat{\sigma}^{1/2}-\sigma_0^{1/2}\|\|_2$	moment $\|\|\tilde{\sigma}^{1/2}-\sigma_0^{1/2}\|\|_2$	#true edges
250	40	0.0317	0.0350	2.3869	2.2941	206.3200
		(0.0043)	(0.0050)	(0.0185)	(0.0179)	(13.5011)
250	60	0.0196	0.0231	2.3886	2.2447	474.0400
		(0.0023)	(0.0029)	(0.0146)	(0.0149)	(22.0247)
250	100	0.0097	0.0140	2.3905	2.1449	1316.9200
		(0.0015)	(0.0019)	(0.0118)	(0.0126)	(33.0795)
500	40	0.0317	0.0350	0.9881	0.9226	206.3200
		(0.0043)	(0.0050)	(0.0131)	(0.0126)	(13.5011)
500	60	0.0196	0.0231	0.9891	0.8874	474.0400
		(0.0023)	(0.0029)	(0.0103)	(0.0106)	(22.0247)
500	100	0.0097	0.0140	0.9903	0.8167	1316.9200
		(0.0015)	(0.0019)	(0.0083)	(0.0089)	(33.0795)
1000	40	0.0317	0.0350	0.0375	0.0615	206.3200
		(0.0043)	(0.0050)	(0.0062)	(0.0076)	(13.5011)
1000	60	0.0196	0.0231	0.0301	0.0794	474.0400
		(0.0023)	(0.0029)	(0.0046)	(0.0071)	(22.0247)
1000	100	0.0097	0.0140	0.0221	0.1255	1316.9200
		(0.0015)	(0.0019)	(0.0034)	(0.0063)	(33.0795)

Table 4: Model selection performance of penalized composite likelihood based on 100 simulated datasets under each setting

n	p	#zero edge	#true edges	fn	fp	tuning parameter
250	40	651.6300	120.5500	27.8200	0.0000	1.2770
		7.7429	12.9008	(10.2152)	(0.0000)	(0.3194)
250	60	1469.2300	323.0300	2.3000	5.4400	1.4985
		19.5349	16.4890	(11.4111)	(19.2518)	(0.2514)
500	40	651.6300	121.4700	26.9000	0.0000	1.2650
		7.7429	13.2432	(10.6520)	(0.0000)	(0.3705)
500	60	1474.0900	325.3300	0.0000	0.5800	1.0910
		13.6929	11.7903	(0.0000)	(5.8000)	(0.1961)

Figure 1: Estimated between-cluster edges for treatment and control groups



Numbers in parenthesis indicate the cluster IDs, followed by the estimated $\hat{\theta}_{E_s}$ for the control and treatment groups.