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Supplementary for Compositional Data Network Analysis via Lasso Penalized D-Trace Loss

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Abstract

Supplementary: The technical details for derivation of Algorithm 1 are summarized in this supplementary. The networks constructed with CD-trace, gCoda, S-E(glasso) and S-E (mb) for Control, Healthy and EBA group in real data analysis are presented in Fig. S1, Fig. S2 and Fig. S3, respectively.
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1 Technical Details for Algorithm 1

Here, we give the details in the derivation of our ADMM algorithm. Since the objective function in (12) is convex, taking the partial derivative with respect to Θ_1 and setting it as zero, we get

$$F\Theta_1 F\hat{\Sigma}_{\ln \boldsymbol{x}}F/2+3\rho\Theta_1-\rho(\Theta_3^k+\Theta_2^k+\Theta_4^k)-F/2-\Lambda_1^k+\Lambda_3^k-\Lambda_4^k=0. \tag{S1}$$

Solving this is equivalent to solving the equation of the form

$$AXB+\gamma X=C, \tag{S2}$$

where A and B are symmetric, nonnegative definite matrices, $\gamma > 0$ is a constant and C is a matrix. Explicit solution to equation (S2) is given by the following Lemma.

Lemma 1. *Let $A = U_A\Sigma_A U_A^T$ and $B = U_B\Sigma_B U_B^T$ be the eigenvalue decompositions of the symmetric matrices A and B, respectively. Assume that $G(A, B, C, \gamma)$ is the solution to (S2). Then, $G(A, B, C, \gamma) = U_A[D \circ (U_A^T C U_B)]U_B^T$, where $D_{ij} = (\sigma_i^A\sigma_j^B + \gamma)^{-1}$ and $\circ$ denotes the Hadamard product of two matrices.*

The above Lemma can be verified by plugging $G(A, B, C, \rho)$ into equation (S2) with some basic calculations. According to this Lemma, the solution to (S1) can be written as

$$\Theta_1^{k+1} = G(F, F\hat{\Sigma}_{\ln \boldsymbol{x}}F, 2\rho\Theta_3^k + 2\rho\Theta_2^k + 2\rho\Theta_4^k + F + 2\Lambda_1^k - 2\Lambda_3^k + 2\Lambda_4^k, 6\rho).$$

Similarly, the solution to (13) is

$$\Theta_2^{k+1} = G(F\hat{\Sigma}_{\ln \boldsymbol{x}}F, F, 2\rho\Theta_3^k + 2\rho\Theta_1^{k+1} + 2\rho\Theta_4^k + F + 2\Lambda_3^k - 2\Lambda_2^k - 2\Lambda_5^k, 6\rho).$$

Leaving out the constant terms in the objective function of (14), it is equivalent to solve

$$\operatorname*{argmin}_{\Delta_3} \rho\|\Theta_3\|_F^2 - <\Theta_3, \rho\Theta_1^{k+1}+\rho\Theta_2^{k+1}-\Lambda_1^k+\Lambda_2^k> +\lambda\|\Theta_3\|_{1,\text{off}}.$$

Given a matrix A and $\lambda > 0$, let $S(A, \lambda)$ be the solution to the following optimization problem

$$S(A,\lambda) = \operatorname*{argmin}_{\Theta} \frac{1}{2}\|\Theta\|_F^2 - <\Theta, A> +\lambda\|\Theta\|_{1,\text{off}}.$$

It is easy to check that the (i, j)th component of $S(A, \lambda)$ $(i \neq j)$ is

$$S(A,\lambda)_{i,j} = \begin{cases} A_{i,j}-\lambda, & A_{i,j} > \lambda, \\ A_{i,j}+\lambda, & A_{i,j} < -\lambda, \\ 0, & -\lambda \le A_{i,j} \le \lambda. \end{cases}$$

Thus the solution to (14) is

$$\Theta_3^{k+1} = S((\rho\Theta_1^{k+1} + \rho\Theta_2^{k+1} - \Lambda_1^k + \Lambda_2^k)/2\rho, \lambda/2\rho).$$

To update Θ_4, we rewrite (15) as

$$\operatorname*{argmin}_{\Theta_4 \succeq \epsilon I} \rho\|\Theta_4\|_F^2 - <\Theta_4, \rho\Theta_1^{k+1} + \rho\Theta_2^{k+1} - \Lambda_4^k + \Lambda_5^k> .$$

Following the idea of Zhang and Zou (2014), we define a matrix operator $[X]_+$ for a symmetric matrix X: let the eigenvalue decomposition of X

be $U_X \,\mathrm{diag}(\lambda_1, \ldots, \lambda_p) U_X^T$, then

$$[X]_+ = U_X \,\mathrm{diag}\{\max(\lambda_1, \epsilon), \ldots, \max(\lambda_p, \epsilon)\} U_X^T.$$

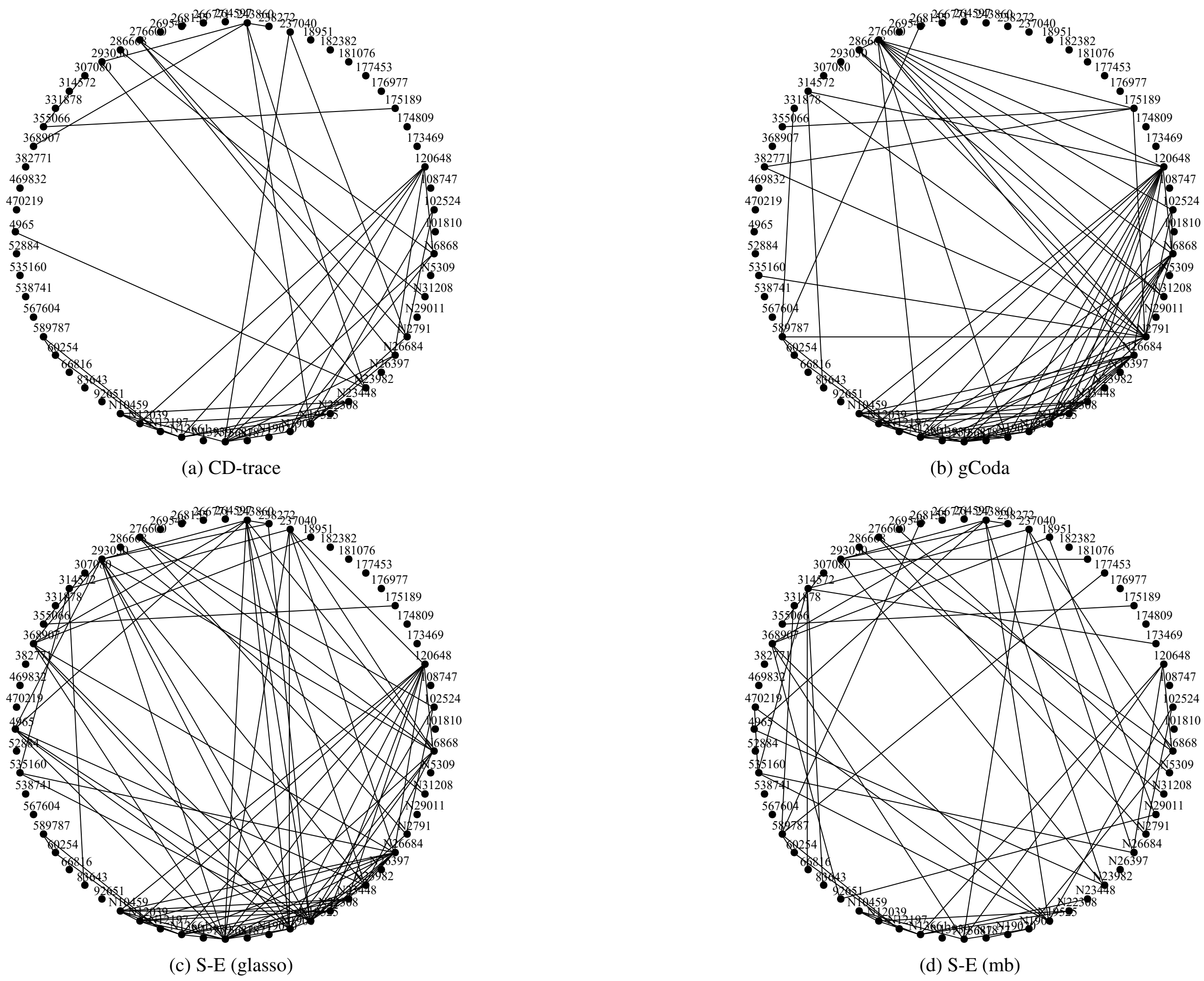
Then the solution to (15) is

$$\Theta_4^{k+1} = [\frac{\rho\Theta_1^{k+1} + \rho\Theta_2^{k+1} - \Lambda_4^k + \Lambda_5^k}{2\rho}]_+$$

Since the update of $\Lambda_i, i = 1, 2, 3, 4, 5$ is trivial, we now have all the pieces needed to carry out the alternating direction method. This AMD algorithm has been summarized in Algorithm 1.

2 Networks Constructed in Real Data Analysis

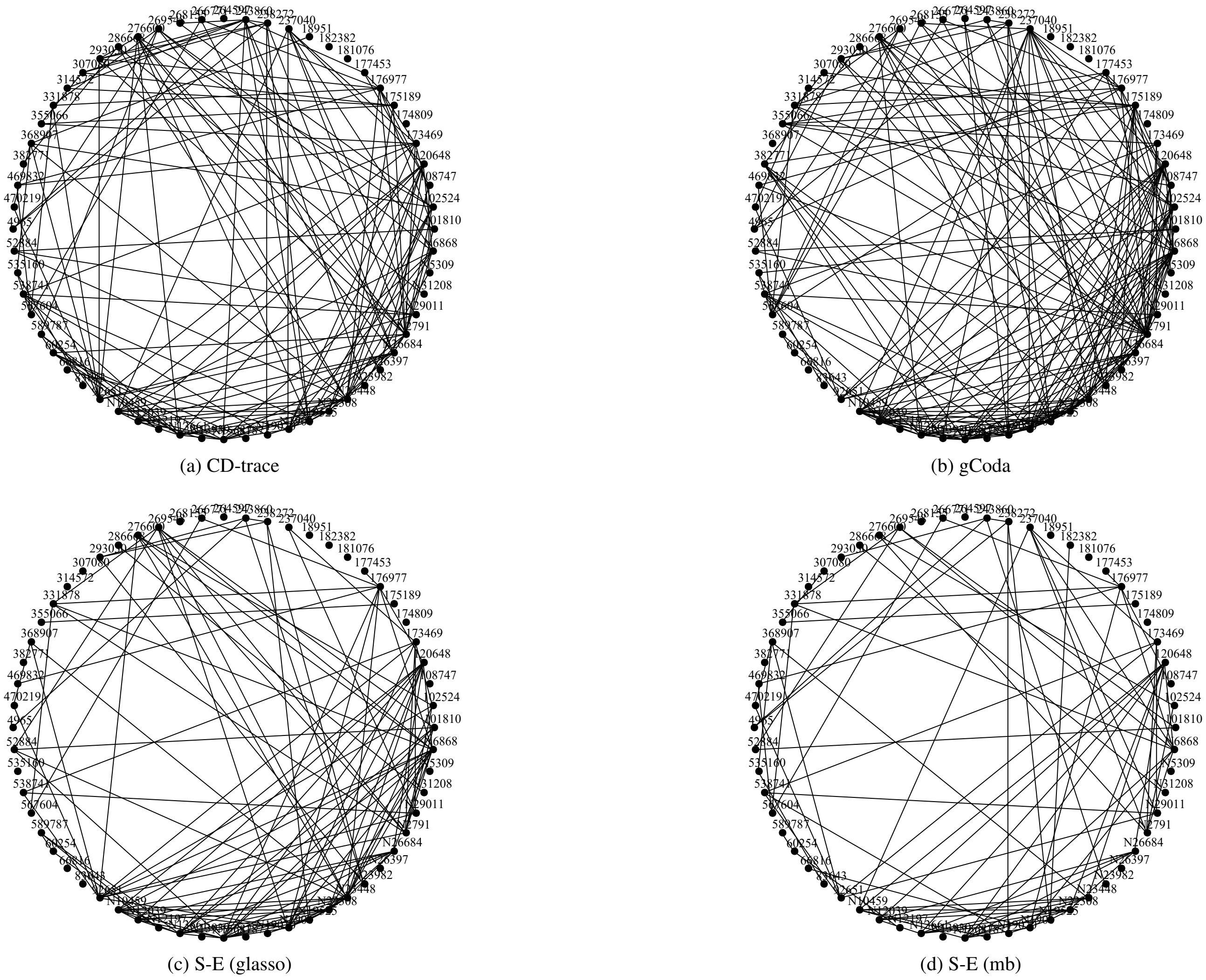
The networks constructed with CD-trace, gCoda, S-E(glasso) and S-E (mb) for Control, Healthy and EBA group in real data analysis are presented in Fig. S1, Fig. S2 and Fig. S3, respectively.



(a) CD-trace (b) gCoda

(c) S-E (glasso) (d) S-E (mb)

Fig. S1. The networks constructed with different methods for Control group.



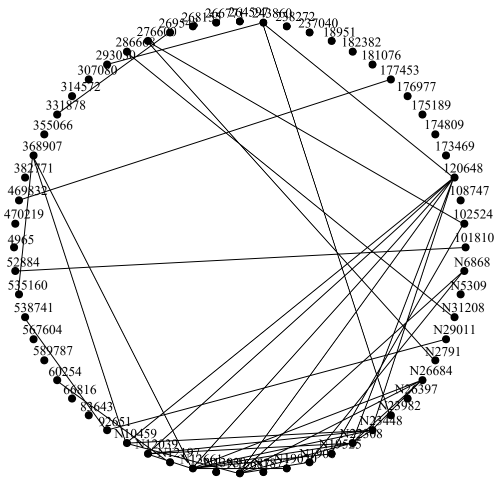
(a) CD-trace

(b) gCoda

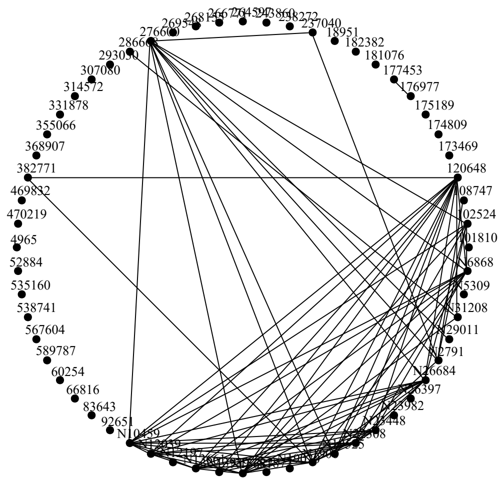
(c) S-E (glasso)

(d) S-E (mb)

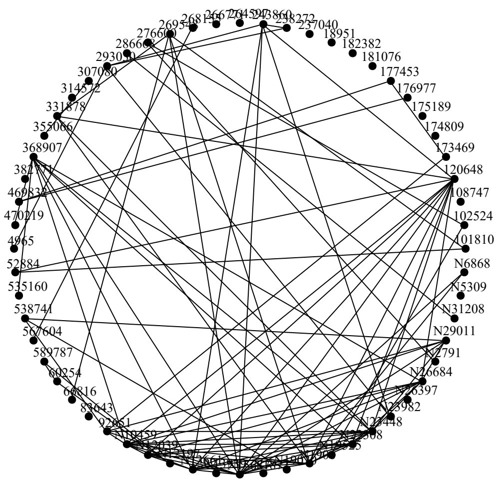
Fig. S2. The networks constructed with different methods for Healthy group.



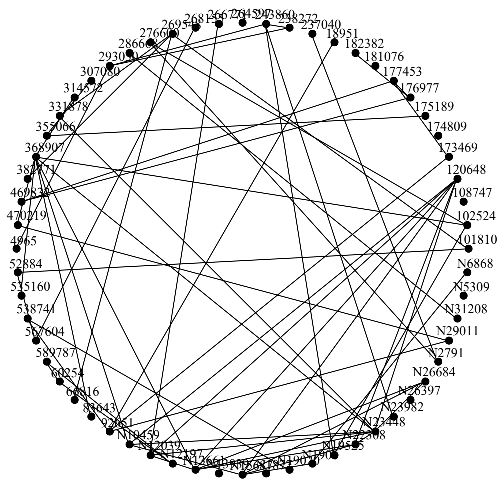
(a) CD-trace



(b) gCoda



(c) S-E (glasso)



(d) S-E (mb)

Fig. S3. The networks constructed with different methods for EBA group.