6 Appendix

6.1 Proof of Lemma 3.1

Sketch of proof: We use change of variable $\mathbf{W} = \mathbf{Z}\mathbf{Z}^{\intercal}$. The matrix \mathbf{W} can be decomposed as $\mathbf{Z}\mathbf{Z}^{\intercal}$ where \mathbf{Z} is $p \times K$, if and only if $\mathbf{W} \succeq 0$ and has rank at most K. The constraints $\|\mathbf{Z}\|_2 \leq \tau$, $\|Z_i\|_2 \leq 1$ and $\|\mathbf{Z}\|_F \leq \beta$ are equivalent with the constraints $\mathbf{W} \preceq \tau^2 I$, diag $(\mathbf{W}) \leq 1$ and tr $(\mathbf{W}) \leq \beta^2$, respectively. Also, note that the condition that the regularization parameters of all (i, j) pairs of variables are non-negative is satisfied implicitly. For the diagonal elements, we have the constraint diag $(\mathbf{W}) \leq 1$ explicitly. Without loss of generality, assume i < j. We know $\mathbf{W} \succeq 0$, therefore we achieve: $M = \begin{bmatrix} W_{ii} & W_{ij} \\ W_{ji} & W_{jj} \end{bmatrix} \succeq 0$. Having $W_{ii} \leq 1$ and $W_{jj} \leq 1$, we conclude $W_{ij} = W_{ji} \leq 1$.

6.2 Proof of Lemma 3.3

<u>Sketch of proof</u>: In the Z-step, to estimate Z given Θ using the BCD method, we solve the following problem based on Eq (2):

$$\underset{\mathbf{Z}\in\mathcal{D}}{\operatorname{maximize}} \operatorname{tr}(\mathbf{Z}\mathbf{Z}^{\mathsf{T}}|\boldsymbol{\Theta}|), \tag{14}$$

which is equivalent to:

$$\underset{\mathbf{Z}\in\mathcal{D}}{\operatorname{maximize}}\sum_{i,j} (\mathbf{Z}\mathbf{Z}^{\mathsf{T}})_{ij} |\Theta_{ij}|, \tag{15}$$

where \mathcal{D} is defined based on the two constraints (a) and (b) described above. First, note that by solving Eq (14), we will have $||Z_i||_2 = 1$, for all variables *i*. Hence, because of the binary assumption, each row of Z will have exactly one element with value 1 and the other elements will be 0.

Then, Eq (15) leads to:

$$\underset{\mathbf{Z}\in\mathcal{D}}{\text{maximize}} \quad \sum_{(i,j)\in\mathcal{F}_Z} |\Theta_{ij}|,$$

which is equivalent to

$$\underset{\mathbf{Z}\in\mathcal{D}}{\text{minimize}} \quad \sum_{(i,j)\notin\mathcal{F}_{\mathbf{Z}}} |\Theta_{ij}|, \tag{16}$$

where \mathcal{F}_Z is the set of edges within blocks B_1, \ldots, B_K : $\mathcal{F}_Z = \bigcup_{k=1}^K \{(i, j) | i, j \in B_k\}$. None of the blocks B_k for all k would be empty due to the constraint (b). Therefore, Eq (16) is equivalent with the K-way graph-cut problem on the similarity matrix $|\Theta|$.

Therefore, in the special case with constraints (a) and (b), **Z**-step is *K*-way graph-cut on $|\Theta|$. The GRAB algorithm can be viewed as an iterative BCD method that 1) uses graph-cut as a clustering method to find **Z** based on $|\Theta|$ as a similarity matrix, and 2) learns a network structure of the GGM by solving graphical lasso problem to find Θ .