1 Cone programming for A-optimal

The A-optimal is cast as the following SDP.

$$\min \sum_{i=1}^{K} u_i \tag{1}$$

subject to

$$n_{ij} \geq 0 \ \forall \{(i,j) | 1 \leq i \leq j \leq K\}, \tag{2}$$

$$\sum_i n_{ii} + \sum_{i<j} n_{ij} = N, \tag{3}$$

and

$$\begin{pmatrix} F(\{n_{ab}\}) & \vec{e}_i \\ \vec{e}_i^t & u_i \end{pmatrix} \geq 0 \text{ for } i = 1, 2, \ldots, K \tag{4}$$

where

$$F(\{n_{ab}\}) = \sum_{a=1}^{K} V_{aa} n_{aa} + \sum_{a<b} V_{ab} n_{ab} \tag{5}$$

with sparse matrices V_{aa} and V_{ab} defined by

$$\begin{aligned} V_{aa;\alpha\beta} &= s_{aa}^{-2} \delta_{a\alpha} \delta_{a\beta} \\ V_{a\neq b;\alpha\beta} &= s_{ab}^{-2} (\delta_{a\alpha}\delta_{a\beta} + \delta_{b\alpha}\delta_{b\beta} - \delta_{a\alpha}\delta_{b\beta} - \delta_{a\beta}\delta_{b\alpha}) \end{aligned} \tag{6}$$

In the notation of the cone programming, there are $K(K+1)/2+K$ variables for minimization:

$$\begin{aligned} \vec{x} &= (\vec{n}^t; \vec{u}^t)^t \\ &= (n_{11}, n_{12}, \ldots, n_{1K}, n_{22}, n_{23}, \ldots, n_{K-1\,K}, n_{KK}, u_1, u_2, \ldots, u_K)^t \end{aligned} \tag{7}$$

The coefficients are

$$\vec{c} = (0, 0, \ldots, 0, 1, 1, \ldots, 1)^t \tag{8}$$

with $K(K+1)/2$ entries of 0s and K entries of 1s.

$$A = (1, 1, \ldots, 1, 0, 0, \ldots, 0) \tag{9}$$

with $K(K+1)/2$ entries of 1s and K entries of 0s.

$$G = -\begin{pmatrix} & I_{K(K+1)/2} & & & 0_{K(K+1)/2,K} & \\ \text{vec}(V_{11}^+) & \text{vec}(V_{12}^+) & \cdots \text{vec}(V_{KK}^+) & \text{vec}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & 0 & \cdots \\ \text{vec}(V_{11}^+) & \text{vec}(V_{12}^+) & \cdots \text{vec}(V_{KK}^+) & 0 & \text{vec}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & \cdots \\ & & & \cdots & & \\ \text{vec}(V_{11}^+) & \text{vec}(V_{12}^+) & \cdots \text{vec}(V_{KK}^+) & 0 & \cdots & \text{vec}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} \tag{10}$$

where

$$V_{ij}^{+} = \begin{pmatrix} V_{ij} & 0 \\ 0 & 0 \end{pmatrix} \tag{11}$$

$$h = \begin{pmatrix} \vec{0}_{K(K+1)/2} \\ \mathrm{vec}\begin{pmatrix} F(\{n^{(0)}\}) & \vec{e}_1 \\ \vec{e}_1^{\,t} & 0 \end{pmatrix} \\ \mathrm{vec}\begin{pmatrix} F(\{n^{(0)}\}) & \vec{e}_2 \\ \vec{e}_2^{\,t} & 0 \end{pmatrix} \\ \vdots \\ \mathrm{vec}\begin{pmatrix} F(\{n^{(0)}\}) & \vec{e}_K \\ \vec{e}_K^{\,t} & 0 \end{pmatrix} \end{pmatrix} \tag{12}$$

The dimensions of the cone programming is

$$\mathrm{dims} = \begin{cases} \text{'l'}: & K(K+1)/2 \\ \text{'q'}: & [\;] \\ \text{'s'}: & [K+1, K+1, \ldots, K+1] \end{cases} \tag{13}$$

G is a VERY sparse matrix of $K(K+1)/2 + K(K+1)^2$ rows and $K(K+1)/2+K$ columns, with highly structured entries. Solving the cone programming for large K requires exploiting the structure in the problem.

We need to solve the KKT equations

$$\begin{pmatrix} 0 & A^t & G^t \\ A & 0 & 0 \\ G & 0 & -W^tW \end{pmatrix} \begin{pmatrix} \vec{x} \\ y \\ \vec{z} \end{pmatrix} = \begin{pmatrix} \vec{p} \\ q \\ \vec{l} \end{pmatrix} \tag{14}$$

$\vec{x}$ and $\vec{p}$ are vectors of length $K(K+1)/2 + K$. We will write

$$\begin{aligned} \vec{x} &= (n_{11}, n_{12}, \ldots, n_{KK}; u_1, u_2, \ldots, u_K)^t \\ \vec{p} &= (p_{11}, p_{12}, \ldots, p_{KK}; \pi_1, \pi_2, \ldots, \pi_K)^t \end{aligned} \tag{15}$$

y and q are two scalar numbers.

$\vec{z}$ and $\vec{l}$ are vectors of length $K(K+1)/2 + K(K+1)^2$. We denote

$$\begin{aligned} \vec{z} &= (z_{11}, z_{12}, \ldots, z_{KK}, \mathrm{vec}(\tilde{z}_1)^t, \mathrm{vec}(\tilde{z}_2)^t, \ldots, \mathrm{vec}(\tilde{z}_K)^t)^t \\ \vec{l} &= (l_{11}, l_{12}, \ldots, l_{KK}, \mathrm{vec}(\tilde{l}_1)^t, \mathrm{vec}(\tilde{l}_2)^t, \ldots, \mathrm{vec}(\tilde{l}_K)^t)^t \end{aligned} \tag{16}$$

where each $\tilde{z}_i$ and $\tilde{l}_i$ is a $K+1$ by $K+1$ square symmetric matrix. We will write $\tilde{z}_i$ in a block form

$$\tilde{z}_i = \begin{pmatrix} \tilde{z}_i^* & \zeta_i \\ \zeta_i^t & z_{i,K+1,K+1} \end{pmatrix} \tag{17}$$

W is a block diagonal matrix, satisfying

$$W^t W \vec{z} = \left(\begin{array}{c} d_{11}^2 z_{11} \\ d_{12}^2 z_{12} \\ \vdots \\ d_{KK}^2 z_{KK} \\ \mathrm{vec}(r_1 r_1^t \tilde{z}_1 r_1 r_1^t) \\ \mathrm{vec}(r_2 r_2^t \tilde{z}_2 r_2 r_2^t) \\ \vdots \\ \mathrm{vec}(r_K r_K^t \tilde{z}_K r_K r_K^t) \end{array} \right) \tag{18}$$

The first group of KKT equations, $A^t y + G^t \vec{x} = \vec{p}$, are

$$y - z_{ab} - \mathrm{vec}(V_{ab})^t \cdot \mathrm{vec}(\sum_i \tilde{z}_i^*) = p_{ab} \text{ for } 1 \le a \le b \le K \tag{19}$$

and

$$-z_{i,K+1,K+1} = \pi_i \text{ for } i = 1, 2, \ldots, K \tag{20}$$

There is only one equation for the second group $A\vec{x} = q$:

$$\sum_a n_{aa} + \sum_{a<b} n_{ab} = q \tag{21}$$

The third group of KKT equations, $G\vec{x} - W^t W \vec{z} = \vec{s}$, are

$$-n_{ab} - d_{ab}^2 z_{ab} = l_{ab} \text{ for } 1 \le a \le b \le K \tag{22}$$

and

$$-\left(\begin{array}{cc} F(\{n_{ab}\}) & 0 \\ 0 & u_i \end{array} \right) - r_i r_i^t \tilde{z}_i r_i r_i^t = \tilde{l}_i \tag{23}$$

Eq. 23 represents $K(K+1)^2$ equations.

We will first eliminate the variables in $\tilde{z}_i^*$. Denoting

$$R_i = r_i^{-t} r_i^{-1} = \left(\begin{array}{cc} R_i^* & \gamma_i \\ \gamma_i^t & R_{i,K+1,K+1} \end{array} \right) \tag{24}$$

Eq. 23 can be rewritten as

$$R_i \left(\begin{array}{cc} F(\{n_{ab}\}) & 0 \\ 0 & u_i \end{array} \right) R_i + \tilde{z}_i = -R_i \tilde{l}_i R_i \tag{25}$$

Writing $L_i \equiv R_i \tilde{l}_i R_i$ in block form

$$L_i = \left(\begin{array}{cc} L_i^* & \lambda_i \\ \lambda_i^t & L_{i,K+1,K+1} \end{array} \right) \tag{26}$$

Eq. 25 becomes

$$R_i^* F(\{n_{ab}\}) R_i^* + \gamma_i \gamma_i^t u_i + \tilde{z}_i^* = -L_i^* \tag{27}$$

$$R_i^* F(\{n_{ab}\})\gamma_i + \gamma_i R_{i,K+1,K+1} u_i + \zeta_i = -\lambda_i \tag{28}$$

and

$$\gamma_i^t F(\{n_{ab}\})\gamma_i + R_{i,K+1,K+1}^2 u_i + z_{i,K+1,K+1} = -L_{i,K+1,K+1} \tag{29}$$

Because $z_{i,K+1,K+1} = -\pi_i$, the last equation is

$$\gamma_i^t F(\{n_{ab}\})\gamma_i + R_{i,K+1,K+1}^2 u_i = \pi_i - L_{i,K+1,K+1} \tag{30}$$

Eq. 27 and Eq. 19 together lead to

$$z_{\alpha\beta} = y - p_{\alpha\beta} + \mathrm{vec}(V_{\alpha\beta})^t \cdot \mathrm{vec}\left(\sum_i R_i^* F(\{n_{ab}\}) R_i^* + \sum_i \gamma_i \gamma_i^t u_i\right) + \mathrm{vec}(V_{\alpha\beta})^t \cdot \mathrm{vec}\left(\sum_i L_i^*\right) \tag{31}$$

Plugging the above in Eq. 22, we also eliminate z_{ab}.

$$\begin{aligned} & d_{\alpha\beta}^{-2} n_{\alpha\beta} + \mathrm{vec}(V_{\alpha\beta})^t \cdot \mathrm{vec}\left(\sum_i R_i^* F(\{n_{ab}\}) R_i^* + \sum_i \gamma_i \gamma_i^t u_i\right) + y \\ = \; & p_{\alpha\beta} - \mathrm{vec}(V_{\alpha\beta})^t \cdot \mathrm{vec}\left(\sum_i L_i^*\right) - d_{\alpha\beta}^{-2} l_{\alpha\beta} \end{aligned} \tag{32}$$

Eq. 32 ($K(K+1)/2$ equations), Eq. 21 (1 equation), and Eq. 30 (K equations) together determine the variables $\{n_{ab}\}$ ($K(K+1)/2$ variables), $\{u_i\}$ (K variables), and y (1 variable).

The matrix of the form $RF(\{n_{ab}\})R$ is

$$\begin{aligned} RF(\{n_{ab}\})R &= \sum_a RV_{aa}Rn_{aa} + \sum_{a<b} RV_{ab}Rn_{ab} \\ &= \sum_a s_{aa}^{-2} R_a R_a^t n_{aa} + \sum_{a<b} s_{ab}^{-2}(R_a R_a^t + R_b R_b^t - R_a R_b^t - R_b R_a^t) n_{ab} \end{aligned} \tag{33}$$

where R_a is the column vector of the ath column of R.

The vector of the form $RF(\{n_{ab}\})\gamma$ is

$$RF(\{n_{ab}\})\gamma = \sum_a s_{aa}^{-2} R_a \gamma_a n_{aa} + \sum_{a<b} s_{ab}^{-2}(R_a\gamma_a + R_b\gamma_b - R_a\gamma_b - R_b\gamma_a) n_{ab} \tag{34}$$

The scalar of the form $\gamma^t F(\{n_{ab}\})$ is

$$\gamma^t F(\{n_{ab}\})\gamma = \sum_a s_{aa}^{-2}\gamma_a^2 n_{aa} + \sum_{a<b} s_{ab}^{-2}(\gamma_a^2 + \gamma_b^2 - 2\gamma_a\gamma_b) n_{ab} \tag{35}$$

The inner product $\mathrm{vec}(V_{\alpha\beta})^t \cdot \mathrm{vec}(X)$ is

$$\mathrm{vec}(V_{\alpha\beta})^t \cdot \mathrm{vec}(X) = \begin{cases} s_{\alpha\alpha}^{-2} X_{\alpha\alpha} & \text{if } \alpha = \beta \\ s_{\alpha\beta}^{-2}\left(X_{\alpha\alpha} + X_{\beta\beta} - X_{\alpha\beta} - X_{\beta\alpha}\right) & \text{if } \alpha \neq \beta \end{cases} \tag{36}$$

The equation for $\{n_{ab}\}$, $\{u_i\}$, and y, summarizing Eq. 32, 21, and 30, is

$$\begin{pmatrix} B & \vec{\eta} \\ \vec{\eta}^t & 0 \end{pmatrix} \begin{pmatrix} \vec{x} \\ y \end{pmatrix} = \begin{pmatrix} \vec{x}_0 \\ y_0 \end{pmatrix} \tag{37}$$

where $\vec{x} = (n_{11}, n_{12}, \ldots, n_{22}, n_{23}, \ldots, n_{KK}, u_1, u_2, \ldots u_K)^t$, and B is a symmetric matrix

$$B = \begin{pmatrix} A & \vec{\eta} \\ \vec{\eta}^t & \mathrm{diag}(R^2_{i,K+1,K+1}) \end{pmatrix} \tag{38}$$

where $\vec{\eta} = (1, 1, ...1, 0, 0, ...0)^t$ is $K(K+1)/2$ 1's followed by K 0's.

Eq. 37 can be solved by

$$\begin{aligned} y &= \frac{\vec{\eta}^t \cdot B^{-1} \cdot \vec{x}_0 - y_0}{\vec{\eta}^t \cdot B^{-1} \vec{\eta}} \\ \vec{x} &= B^{-1}\vec{x}_0 - yB^{-1}\vec{\eta} \end{aligned} \tag{39}$$

Some algebra shows that the first $K(K+1)/2$-by-$K(K+1)/2$ submatrix of A is given by

$$A_{\alpha\beta,ab} = s_{ab}^{-2} s_{\alpha\beta}^{-2} \cdot \begin{cases} \sum_i R^2_{i,a,\alpha} & \text{if } a = b, \alpha = \beta \\ \sum_i (R_{i,a,\alpha} - R_{i,b,\alpha})^2 & \text{if } a \neq b, \alpha = \beta \\ \sum_i (R_{i,a,\alpha} - R_{i,a,\beta})^2 & \text{if } a = b, \alpha \neq \beta \\ \sum_i ((R_{i,a,\alpha} - R_{i,b,\alpha}) - (R_{i,a,\beta} - R_{i,b,\beta}))^2 & \text{if } a \neq b, \alpha \neq \beta \end{cases} \tag{40}$$

The computation of this submatrix $A_{\alpha\beta,ab}$ is $O(K^5)$ in time complexity and $O(K^4)$ in memory complexity; it is the most intensive computation in computing the A-optimal by cone programming.