

# 1 Cone programming for A-optimal

The A-optimal is cast as the following SDP.

$$\min \sum_{i=1}^K u_i \quad (1)$$

subject to

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

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

and

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

where

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

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

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

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

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

The coefficients are

$$\vec{c} = (0, 0, \dots, 0, 1, 1, \dots, 1)^t \quad (8)$$

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

$$A = (1, 1, \dots, 1, 0, 0, \dots, 0) \quad (9)$$

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

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

where

$$V_{ij}^+ = \begin{pmatrix} V_{ij} & 0 \\ 0 & 0 \end{pmatrix} \quad (11)$$

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

The dimensions of the cone programming is

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

$G$  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

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

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

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

$y$  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

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

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

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

$W$  is a block diagonal matrix, satisfying

$$W^t W \vec{z} = \begin{pmatrix} d_{11}^2 z_{11} \\ d_{12}^2 z_{12} \\ \vdots \\ d_{KK}^2 z_{KK} \\ \text{vec}(r_1 r_1^t \tilde{z}_1 r_1 r_1^t) \\ \text{vec}(r_2 r_2^t \tilde{z}_2 r_2 r_2^t) \\ \vdots \\ \text{vec}(r_K r_K^t \tilde{z}_K r_K r_K^t) \end{pmatrix} \quad (18)$$

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

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

and

$$-z_{i,K+1,K+1} = \pi_i \text{ for } i = 1, 2, \dots, K \quad (20)$$

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

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

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

$$-n_{ab} - d_{ab}^2 z_{ab} = l_{ab} \text{ for } 1 \leq a \leq b \leq K \quad (22)$$

and

$$-\begin{pmatrix} F(\{n_{ab}\}) & 0 \\ 0 & u_i \end{pmatrix} - r_i r_i^t \tilde{z}_i r_i r_i^t = \tilde{l}_i \quad (23)$$

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

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

$$R_i = r_i^{-t} r_i^{-1} = \begin{pmatrix} R_i^* & \gamma_i \\ \gamma_i^t & R_{i,K+1,K+1} \end{pmatrix} \quad (24)$$

Eq. 23 can be rewritten as

$$R_i \begin{pmatrix} F(\{n_{ab}\}) & 0 \\ 0 & u_i \end{pmatrix} R_i + \tilde{z}_i = -R_i \tilde{l}_i R_i \quad (25)$$

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

$$L_i = \begin{pmatrix} L_i^* & \lambda_i \\ \lambda_i^t & L_{i,K+1,K+1} \end{pmatrix} \quad (26)$$

Eq. 25 becomes

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

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

and

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

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

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

Eq. 27 and Eq. 19 together lead to

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

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

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

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

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

where  $R_a$  is the column vector of the  $a$ th column of  $R$ .

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

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

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

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

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

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

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

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

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

$$B = \begin{pmatrix} A & \vec{\eta} \\ \vec{\eta}^t & \text{diag}(R_{i,K+1,K+1}^2) \end{pmatrix} \quad (38)$$

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

Eq. 37 can be solved by

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

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

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

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.

## 2 Including reference input

Often, some of the quantities, say  $\{x_a | a \in Q\}$ , are measured by other experiments to within certain statistical error  $\{\hat{x}_a \pm \delta_a | a \in Q\}$ . The likelihood that our new measurements produce the set of values  $\{\hat{x}_e\}$  and the other experiments produce the set of values  $\{\hat{x}_a | a \in Q\}$ , given the true values of the quantities of  $\{x_i\}$ , is

$$\begin{aligned} L &= \prod_i (\sqrt{2\pi\sigma_i})^{-1} \exp\left(-\frac{(x_i - \hat{x}_i)^2}{2\sigma_i^2}\right) \\ &\cdot \prod_{a \in Q} (\sqrt{2\pi\delta_a})^{-1} \exp\left(-\frac{(x_a - \tilde{x}_a)^2}{2\delta_a^2}\right) \\ &\cdot \prod_{i < j} (\sqrt{2\pi\sigma_{ij}})^{-1} \exp\left(-\frac{(x_i - x_j - \hat{x}_{ij})^2}{2\sigma_{ij}^2}\right) \end{aligned} \quad (41)$$

Maximizing  $\ln L$  with respect to  $\{x_i\}$  yields

$$F\vec{x} = \vec{z} \quad (42)$$

where

$$F_{ij} = \begin{cases} \delta_i^{-2} + \sigma_i^{-2} + \sum_{k \neq i} \sigma_{ik}^{-2} & \text{if } i = j \text{ and } i \in Q \\ \sigma_i^{-2} + \sum_{k \neq i} \sigma_{ki}^{-2} & \text{if } i = j \text{ and } i \notin Q \\ -\sigma_{ij}^{-2} & \text{if } i \neq j \end{cases} \quad (43)$$

and

$$z_i = \begin{cases} \sigma_i^{-2} \hat{x}_i + \delta_i^{-2} \tilde{x}_i + \sum_{j \neq i} \sigma_{ij}^{-2} \hat{x}_{ij} & \text{if } i \in Q \\ \sigma_i^{-2} \hat{x}_i + \sum_{j \neq i} \sigma_{ij}^{-2} & \text{if } i \notin Q \end{cases} \quad (44)$$