Appendix A
Solution to Problem 21

By introducing an auxiliary variable $\boldsymbol{\nu}$, Problem 21 can be further rewritten as follows.

$$\begin{aligned} &\min_{\boldsymbol{\mu},\boldsymbol{\nu}} \boldsymbol{\mu}^T \mathbf{M}\boldsymbol{\nu} + 2\boldsymbol{\mu}^T \mathbf{y} \\ &s.t.\ \boldsymbol{\mu}^T \mathbf{1} = 1, \boldsymbol{\mu} \geq \mathbf{0}, \boldsymbol{\mu} = \boldsymbol{\nu} \end{aligned} \tag{1}$$

So, we have the following augmented Lagrangian function.

$$\begin{aligned} &\min_{\boldsymbol{\mu},\boldsymbol{\nu}} \boldsymbol{\mu}^T \mathbf{M}\boldsymbol{\nu} + 2\boldsymbol{\mu}^T \mathbf{y} + \frac{\rho}{2}\left\|\boldsymbol{\mu} - \boldsymbol{\nu} + \frac{\boldsymbol{\eta}}{\rho}\right\|_2^2 \\ &s.t.\ \boldsymbol{\mu}^T \mathbf{1} = 1, \boldsymbol{\mu} \geq \mathbf{0} \end{aligned} \tag{2}$$

where ρ is the penalty parameter and $\boldsymbol{\eta}$ is the Lagrangian multiplier. Next alternate optimization will be performed. **Step 1**: Fixing $\boldsymbol{\mu}$, we have

$$\min_{\boldsymbol{\nu}} \boldsymbol{\mu}^T \mathbf{M}\boldsymbol{\nu} + \frac{\rho}{2}\left\|\boldsymbol{\mu} - \boldsymbol{\nu} + \frac{\boldsymbol{\eta}}{\rho}\right\|_2^2 \tag{3}$$

Taking derivative and setting it to zero, we know

$$\mathbf{M}^T \boldsymbol{\mu} - \rho(\boldsymbol{\mu} - \boldsymbol{\nu} + \boldsymbol{\eta}/\rho) = 0 \tag{4}$$

The solution is derived as follows.

$$\boldsymbol{\nu} = \boldsymbol{\mu} + (\boldsymbol{\eta} - \mathbf{M}^T \boldsymbol{\mu})/\rho \tag{5}$$

Step 2: Fixing $\boldsymbol{\nu}$, we have

$$\begin{aligned} &\min_{\boldsymbol{\mu}} \boldsymbol{\mu}^T \mathbf{M}\boldsymbol{\nu} + 2\boldsymbol{\mu}^T \mathbf{y} + \frac{\rho}{2}\left\|\boldsymbol{\mu} - \boldsymbol{\nu} + \frac{\boldsymbol{\eta}}{\rho}\right\|_2^2 \\ &s.t.\ \boldsymbol{\mu}^T \mathbf{1} = 1, \boldsymbol{\mu} \geq \mathbf{0} \end{aligned} \tag{6}$$

Eq. (6) is equivalent to the following problem.

$$\begin{aligned} &\min_{\boldsymbol{\mu}} \boldsymbol{\mu}^T \boldsymbol{\mu} - 2\boldsymbol{\mu}^T (\rho\boldsymbol{\nu} - \boldsymbol{\eta} - \mathbf{M}\boldsymbol{\nu} - 2\mathbf{y})/\rho \\ &s.t.\ \boldsymbol{\mu}^T \mathbf{1} = 1, \boldsymbol{\mu} \geq \mathbf{0} \end{aligned} \tag{7}$$

Let $\mathbf{e} = (\rho\boldsymbol{\nu} - \boldsymbol{\eta} - \mathbf{M}\boldsymbol{\nu} - 2\mathbf{y})/\rho$, Eq. (7) can be further rewritten as follows.

$$\begin{aligned} &\min_{\boldsymbol{\mu}} \|\boldsymbol{\mu} - \mathbf{e}\|_2^2 \\ &s.t.\ \boldsymbol{\mu}^T \mathbf{1} = 1, \boldsymbol{\mu} \geq \mathbf{0} \end{aligned} \tag{8}$$

The Lagrangian function of Eq. (8) is

$$\mathcal{L}(\boldsymbol{\mu}, \zeta, \boldsymbol{\xi}) = \frac{1}{2}\|\boldsymbol{\mu} - \mathbf{e}\|_2^2 - \zeta(\boldsymbol{\mu}^T \mathbf{1} - 1) - \boldsymbol{\xi}^T \boldsymbol{\mu} \tag{9}$$

According to the KKT conditions, we have

$$\mu_i^* = \left(z_i - \bar{\xi}^*\right)_+ \tag{10}$$

$$\xi_i^* = \left(\bar{\xi}^* - z_i\right)_+ \tag{11}$$

where $\mathbf{z} = \mathbf{e} - \frac{\mathbf{1}\mathbf{1}^T}{n_v}\mathbf{e} + \frac{\mathbf{1}}{n_v}$ and $\bar{\xi}^* = \frac{\mathbf{1}^T \boldsymbol{\xi}^*}{n_v}$. Obviously, $\boldsymbol{\mu}$ can be determined by Eq. (10) if we know $\bar{\xi}^*$. From Eq. (11), we further know the following relationship.

$$\bar{\xi}^* = \frac{1}{n_v}\sum_{i=1}^{n_v}\left(\bar{\xi}^* - z_i\right)_+ \tag{12}$$

Defining a function as

$$f(\bar{\xi}) = \frac{1}{n_v}\sum_{i=1}^{n_v}\left(\bar{\xi} - z_i\right)_+ - \bar{\xi} \tag{13}$$

we can obtain $\bar{\xi}^*$ by the root-finding problem $f\left(\bar{\xi}^*\right) = 0$. This problem can be solved efficiently by Newton method (14), requiring only 2-4 iterations.

$$\bar{\xi}_{t+1} = \bar{\xi}_t - \frac{f\left(\bar{\xi}_t\right)}{f'\left(\bar{\xi}_t\right)} \tag{14}$$

Step 3: Get a more accurate multiplier by $\boldsymbol{\eta} = \boldsymbol{\eta} + \rho(\boldsymbol{\mu} - \boldsymbol{\nu})$.
Step 4: Increase the penalty parameter by $\rho = \tau\rho$.
In a nutshell, Problem 21 can be solved through the above four steps.

Appendix B
Derivation of Equations 10 and 11

For any i, Eq. (9) has the following KKT conditions:

$$\mu_i^* - e_i - \zeta^* - \xi_i^* = 0 \tag{15}$$

$$\xi_i^* \mu_i^* = 0 \tag{16}$$

$$\mu_i^* \geq 0 \tag{17}$$

$$\xi_i^* \geq 0 \tag{18}$$

According to $\mathbf{1}^T \boldsymbol{\mu}^* = 1$ and Eq. (15), we know

$$\zeta^* = \left(1 - \mathbf{1}^T \mathbf{e} - \mathbf{1}^T \boldsymbol{\xi}^*\right)/n_v \tag{19}$$

Combining Eq. (15) and Eq. (19), we have

$$\mu_i^* = z_i - \bar{\xi}^* + \xi_i^* \tag{20}$$

where $\mathbf{z} = \mathbf{e} - \frac{\mathbf{1}\mathbf{1}^T}{n_v}\mathbf{e} + \frac{\mathbf{1}}{n_v}$ and $\bar{\xi}^* = \frac{\mathbf{1}^T \boldsymbol{\xi}^*}{n_v}$. Following Eqs. (16)-(18) and (20), Eqs. (10) and (11) hold.