Recall: $D_{ij} = K_{ii} + K_{jj} - 2K_{ij}$ ①

Introduce $k = \mathrm{diag}(K) = (K_{11}, K_{22}, \cdots, K_{nn})^T \in \mathbb{R}^n$,

then
$$\underset{n\times 1}{k} \cdot \underset{1\times n}{\mathbb{1}^T} = \begin{pmatrix} K_{11} \\ \vdots \\ K_{nn} \end{pmatrix} (1, \cdots, 1) = \begin{pmatrix} K_{11} & K_{11} & \cdots & K_{11} \\ K_{22} & K_{22} & \cdots & K_{22} \\ \vdots & \vdots & & \vdots \\ K_{nn} & K_{nn} & \cdots & K_{nn} \end{pmatrix}$$

$$\mathbb{1} \cdot k^T = (k \cdot \mathbb{1}^T)^T = \begin{pmatrix} K_{11} & K_{22} & \cdots & K_{nn} \\ K_{11} & K_{22} & \cdots & K_{nn} \\ \vdots & \vdots & & \vdots \\ K_{11} & K_{22} & \cdots & K_{nn} \end{pmatrix}$$

Thus $(k \cdot \mathbb{1}^T)_{ij} = K_{ii}$ and $(\mathbb{1} \cdot k^T)_{ij} = K_{jj}$.

We can write ① as

$$D = k \cdot \mathbb{1}^T + \mathbb{1} \cdot k^T - 2K \quad ②$$

Now suppose $D = (D_{ij})$ is given.

Multiply ② from the right by $\mathbb{1}$:

$$D\mathbb{1} = k\cdot(\mathbb{1}^T\mathbb{1}) + \mathbb{1}\cdot k^T\cdot\mathbb{1} - 2\underbrace{\cancel{K\mathbb{1}}}_{=0}$$

$$= k\cdot\Bigg(\underbrace{(1,\dots,1)\begin{pmatrix}1\\ \vdots\\ 1\end{pmatrix}}_{=n}\Bigg) + \mathbb{1}\cdot k^T\cdot\mathbb{1}$$

$$= nk + \mathbb{1}k^T\mathbb{1} \qquad ③$$

Multiply ③ from the left by $\mathbb{1}^T$:

$$\mathbb{1}^T D\mathbb{1} = n\cdot\mathbb{1}^T k + \underbrace{(\mathbb{1}^T\mathbb{1})}_{n} k^T\mathbb{1}$$

$$= n\cdot\underbrace{\mathbb{1}^T k}_{=(\mathbb{1}\cdot k)} + n\underbrace{k^T\mathbb{1}}_{=(k\cdot\mathbb{1})}$$

$$= 2n\,k^T\mathbb{1}$$

$$\Rightarrow \quad k^T\mathbb{1} = \frac{1}{2n}\,\mathbb{1}^T D\mathbb{1} \qquad ④$$

Insert ④ into ③:

$$D \cdot \mathbb{1} = n k + \mathbb{1}(k^T \mathbb{1})$$

$$\overset{④}{=} n k + \mathbb{1}\left(\frac{1}{2n} \mathbb{1}^T D \mathbb{1}\right)$$

$$= n k + \frac{1}{2n} \mathbb{1} \mathbb{1}^T D \mathbb{1}$$

$$\Rightarrow \quad k = \frac{1}{n} D \cdot \mathbb{1} - \frac{1}{2n^2} \mathbb{1} \mathbb{1}^T D \mathbb{1} \qquad ⑤$$

Insert ⑤ into ②:

$$2K \overset{②}{=} k \cdot \mathbb{1}^T + \mathbb{1} \cdot k^T - D$$

$$\overset{⑤}{=} \left(\frac{1}{n} D \cdot \mathbb{1} - \frac{1}{2n^2} \mathbb{1} \mathbb{1}^T D \mathbb{1}\right) \mathbb{1}^T +$$

$$\mathbb{1} \cdot \left(\frac{1}{n} D \mathbb{1} - \frac{1}{2n^2} \mathbb{1} \mathbb{1}^T D \mathbb{1}\right)^T - D$$

$$= \frac{1}{n} D \cdot \mathbb{1} \mathbb{1}^T - \frac{1}{2n^2} \mathbb{1} \mathbb{1}^T D \mathbb{1} \mathbb{1}^T +$$

$$\frac{1}{n}\mathbb{1}\mathbb{1}^T D - \underbrace{\frac{1}{2n^2}\mathbb{1}\mathbb{1}^T D \mathbb{1}\mathbb{1}^T}_{} - D$$

$$= -D + \frac{1}{n} D \mathbb{1}\mathbb{1}^T + \frac{1}{n}\mathbb{1}\mathbb{1}^T D - \frac{1}{n^2}\mathbb{1}\mathbb{1}^T D \mathbb{1}\mathbb{1}^T$$

$$= -D \underbrace{\left(I - \frac{1}{n}\mathbb{1}\mathbb{1}^T\right)}_{= H \text{ centering matrix}} + \frac{1}{n}\mathbb{1}\mathbb{1}^T D \underbrace{\left(I - \frac{1}{n}\mathbb{1}\mathbb{1}^T\right)}_{= H}$$

$$= -DH + \frac{1}{n}\mathbb{1}\mathbb{1}^T D H$$

$$= -\underbrace{\left(I - \frac{1}{n}\mathbb{1}\mathbb{1}^T\right)}_{= H} DH$$

$$= -HDH$$

$$\Rightarrow \quad K = -\frac{1}{2} HDH$$

This is the representation of K in terms of D.

Back to the MDS problem. Suppose the "artificial features" exist so that the sample pts can be represented as

$$x^{(1)}, \dots, x^{(n)} \in \mathbb{R}^d, \quad \text{then}$$

$$K = X^T X = -\frac{1}{2} HDH \quad \text{is determined.}$$

Eigenvalue decomp of K gives

$$K = V \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} V^T = -\frac{1}{2} HDH$$

where $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$ are the eigenvalues of K

We can take

$$X = \begin{pmatrix} \sqrt{\lambda_1} & & & & \\ & \ddots & & & \\ & & \sqrt{\lambda_d} & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} V^T.$$