1 Original Problem

The original problem is:

$$\min_{S,Y} \| X - ASY \|_F^2$$
s.t. $S^T S = I, S_{ij} \in \{0,1\}, Y_i \in \Omega$ (1)

 Ω is a set in \mathbf{R}^n , it equals to $e_1, e_2, ..., e_n$, where e_i is the i-th column of the identity matrix.

where Y_i is a column of Matrix $\mathbf{Y}, \mathbf{X} \in \mathbf{R}^{Dim \times n}$, $\mathbf{A} \in \mathbf{R}^{Dim \times m}$, $\mathbf{Y} \in \mathbf{R}^{k \times n}$. And \mathbf{S} is the selection matrix, $\mathbf{S} \in \mathbf{R}^{m \times k}, m \geq k$.

2 Relaxed Problem

The original problem is strongly NP-hard and also difficult to solve approximately. It is quite similar to the below one by relax it's constraint:

$$\min_{S,Y} \| X - ASY \|_F^2$$
s.t. $S^T S = I, S \ge 0 Y_i \in \Omega$ (2)

The problem above is equal to:

$$\min_{Y,S,} \quad \|X - DM\|_F^2 \tag{3}$$

s.t.
$$A \cdot S = D$$
, $Y = M$, $S = Q$, $S = J$, $Q^TQ = I$, $J \ge 0$, $Y_i \in \Omega$

where Y_i is a column of Matrix \mathbf{Y} , $\mathbf{X} \in \mathbf{R}^{Dim \times n}$, $\mathbf{A} \in \mathbf{R}^{Dim \times m}$, $\mathbf{Y}, \mathbf{M} \in \mathbf{R}^{k \times n}$. And \mathbf{S} is the selection matrix, $\mathbf{S} \in \mathbf{R}^{m \times k}$, $m \geq k$.

3 Solution

A popular method for this above problem is the Augmented Lagrange Multiplier Method(ALM). The original problem is transformed below:

$$\min_{Y,S,D,Q,J} \| X - DM \|_F^2 + \langle Z_1, S - Q \rangle + \langle Z_2, S - J \rangle
+ \langle Z_3, AS - D \rangle + \langle Z_4, Y - M \rangle
+ \frac{1}{2}\mu \| S - Q \|_F^2 + \frac{1}{2}\mu \| S - J \|_F^2
+ \frac{1}{2}\mu \| AS - D \|_F^2 + \frac{1}{2}\mu \| Y - M \|_F^2
s.t. $Q^TQ = I, J \ge 0, Y_i \in \Omega$$$
(4)

where Y_i is a column of Matrix \mathbf{Y} , $\mathbf{D} \in \mathbf{R}^{Dim \times k}$ and \mathbf{S} , \mathbf{Q} , $\mathbf{J} \in \mathbf{R}^{m \times k}$, $\mathbf{M} \in \mathbf{R}^{k \times n}$.

The ALM can be decomposed into 6 subproblems. All this 6 subproblems have close-formed solutions. So we can do the optimization by 6 steps.

Steps 1: Fix $S, D, Q, J, M, Z_1, Z_2, Z_3, Z_4$ to optimize Y and ignore the constant items, We can get:

$$\min_{Y} \langle Z_4, Y - M \rangle + \frac{1}{2}\mu \| Y - M \|_F^2$$
 (5)
 $s.t. \ Y_i \in \Omega$

$$\min_{Y} \| Y - (M - \frac{Z_4}{\mu}) \|_F^2$$

$$s.t. \ Y_i \in \Omega$$
(6)

 \Longrightarrow

$$Y_{ij} = \begin{cases} 1 & j = t \\ 0 & j \neq t \end{cases}$$
 (7)

where **t** is the index of max member of the i-th column of matrix $\mathbf{M} - \frac{\mathbf{Z_4}}{\mu}$ and $\mathbf{Y_{ij}}$ is the j-th member of i-th column of matrix \mathbf{Y} . Now we get Y.

Steps 2: Fix $S, M, Y, Q, J, Z_1, Z_2, Z_3, Z_4$ to optimize D and ignore the constant items, We can get:

$$\min_{D} \quad \|X - DY\|_{F}^{2} + \langle Z_{3}, AS - D \rangle + \frac{1}{2}\mu \|AS - D\|_{F}^{2}$$
 (8)

We can get the first-order differential of this formulation, and let it to be zero:

$$2(DY - X)Y^{T} - Z_{3} + \mu(D - AS) = 0$$

$$2DY \cdot Y^{T} + \mu D = 2XY^{T} + \mu AS + Z_{3}$$

$$D(2YY^{T} + \mu I) = 2XY^{T} + \mu AS + Z_{3}$$

$$D = (2XY^{T} + \mu AS + Z_{3}) \cdot (2YY^{T} + \mu I)^{-1}$$

Now we can get D.

Steps 3: Fix $D, Y, M, Q, J, Z_1, Z_2, Z_3, Z_4$ to optimize S and ignore the constant items, We can get:

$$\min_{S} \langle Z_{1}, S - Q \rangle + \langle Z_{2}, S - J \rangle + \langle Z_{3}, AS - D \rangle
+ \frac{1}{2}\mu \|S - Q\|_{F}^{2} + \frac{1}{2}\mu \|S - J\|_{F}^{2} + \frac{1}{2}\mu \|AS - D\|_{F}^{2}$$
(9)

We can get the first-order differential of this formulation, and let it to be zero:

$$Z_1 + Z_2 + A^T \cdot Z_3 + \mu(S - Q) + \mu(S - J) + \mu A^T (AS - D) = 0$$

$$2\mu \cdot S + \mu \cdot A^T AS = \mu(A^T D + Q + J) - A^T \cdot Z_3 - Z_1 - Z_2$$

$$S = (2I + A^T A)^{-1} \cdot (A^T D + Q + J) - \frac{1}{\mu} \cdot (A^T \cdot Z_3 + Z_1 + Z_2)$$

Now we can get S.

Steps 4: Fix $D, Y, S, Q, J, Z_1, Z_2, Z_3, Z_4$ to optimize M and ignore the constant items, We can get:

$$\min_{M} \| X - DM \|_{F}^{2} + \langle Z_{4}, Y - M \rangle + \frac{1}{2}\mu \| Y - M \|_{F}^{2}$$
 (10)

We can get the first-order differential of this formulation, and let it to be zero:

$$2D^{T}(DM - X) - Z_4 + \mu(M - Y) = 0$$
$$2D^{T}D \cdot M + \mu M = Z_4 + \mu Y + 2D^{T}X$$
$$M = (2D^{T}D + \mu I)^{-1} \cdot (Z_4 + \mu Y + 2D^{T}X)$$

Now we can get M.

Steps 5: Fix $D, Y, M, S, J, Z_1, Z_2, Z_3, Z_4$ to optimize Q and ignore the constant items, We can get:

$$\min_{Q} \langle Z_1, S - Q \rangle + \frac{1}{2}\mu \| S - Q \|_F^2
s.t. \ Q^T Q = I$$
(11)

It equals to:

$$\min_{Q} \langle Z_1, -Q \rangle - \mu \langle S, Q \rangle
s.t. \ Q^T Q = I$$
(12)

 \iff

$$\max_{Q} \langle Q, \mu S + Z_1 \rangle$$
s.t. $Q^T Q = I$ (13)

Use the proposition of matrix:

The dual norm of the operator norm $\|\cdot\|$ in $R^{m\times n}$ is the nuclear norm $\|\cdot\|_*$.

$$\parallel X \parallel_* := \max_Y \{ < X, Y > \ : \ \parallel Y \parallel \leq 1 \} \tag{14}$$

Now let $X = U\Sigma V^T$ be a **thin** singular value decomposition of the $m\times n$ matrix X,where U is an $m\times n$ matrix and $U^T\cdot U=I$, but $U\cdot U^T\neq I$. V is an $n\times n$ orthogonal matrix which $V\cdot V^T=I$. Σ is an $n\times n$ matrix.Let $Y:=U\cdot V^T, \parallel Y\parallel=1$ and $Tr(Y^T\cdot X)=Tr(VU^T\cdot U\Sigma V^T)=Tr(\Sigma)=\parallel X\parallel_*$. And can get $Y^T\cdot Y=I$.

So from this derivation, We can also do a **thin** singular value decomposition of $\mu S + Z_1$:

$$\mu S + Z_1 = U \Sigma V^T$$
$$Q = U \cdot V^T$$

Steps 6: Fix $D, Y, S, M, Q, Z_1, Z_2, Z_3, Z_4$ to optimize J and ignore the constant items, We can get:

$$\min_{\substack{J \\ s \ t}} \langle Z_2, S - J \rangle + \frac{1}{2}\mu \| S - J \|_F^2 \tag{15}$$

 \iff

$$\min_{J} \frac{2}{\mu} < Z_2, S - J > + ||S - J||_F^2 + \frac{1}{\mu} ||Z_2||_F^2
s.t. J \ge 0$$
(16)

 \leftarrow

$$\min_{J} \| J - (S + \frac{Z_2}{\mu}) \|_F^2
s.t. \ J \ge 0$$
(17)

$$J = \frac{1}{2} \cdot \left[abs(S + \frac{Z_2}{\mu}) + (S + \frac{Z_2}{\mu}) \right]$$
 (18)

Steps 7: Do some updates:

$$Z_{1} = Z_{1} + \mu \cdot (S - Q)$$

$$Z_{2} = Z_{2} + \mu \cdot (S - J)$$

$$Z_{3} = Z_{3} + \mu (AS - D)$$

$$Z_{4} = Z_{4} + \mu (Y - M)$$

$$\mu = \begin{cases} \rho \times \mu & \mu \leq 10^{30} \\ 10^{30} & \text{else} \end{cases}$$
(19)

where $\rho = 1.1$.

4 Termination Conditions

The algorithm will stop when the conditions are both satisfied:

$$\begin{split} \parallel S - Q \parallel_{\infty} < \varepsilon \\ \parallel S - J \parallel_{\infty} < \varepsilon \\ \parallel Y - M \parallel_{\infty} < \varepsilon \end{split} \tag{20}$$

$$\begin{split} \parallel A \cdot S - D \parallel_{F} < \varepsilon \times \parallel A \parallel_{F} \end{split}$$

where $\varepsilon = 10^{-8}$.