single cell biclustering

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1 Objective function

$$
\begin{aligned}
&z : n \times p \\
&X_i : i\text{-th row of} X \\
&X^j : j\text{-th column of} X \\
&\Omega : \{(i,j) : z_{ij} = 0\} \\
&X_\Omega : n \times p \\
s.t. \quad &[X_\Omega]_{ij} = \begin{cases} x_{ij} & \text{if } (i,j) \in \Omega \\ 0 & \text{if } (i,j) \notin \Omega \end{cases}
\end{aligned}
$$

Objective function:

$$
\min_{X \in R^{n\times p}} \frac{1}{2}\|Z - X\|_F^2 + \gamma\|X_\Omega\|_F^2 + \sum_{i<j} P_\lambda(\|X_i - X_j\|) + \sum_{k<l} P_\lambda(\|X^k - X^l\|) \tag{1}
$$

$$
\begin{aligned}
\min_{X \in R^{n\times p}} \frac{1}{2}\|Z - X\|_F^2 + \gamma\|X_\Omega\|_F^2 + \sum_{i<j} P_\lambda(\|A_{ij}\|) + \sum_{k<l} P_\lambda(\|B_{kl}\|) \\
\text{s.t. } X_i - X_j = A_{ij},\ X^k - X^l = B_{kl}
\end{aligned} \tag{2}
$$

Lagrangian form:

$$
\begin{aligned}
L_\delta(X, A, B, U, V) = &\frac{1}{2}\|Z - X\|_F^2 + \gamma\|X_\Omega\|_F^2 + \sum_{i<j} P_\lambda(\|A_{ij}\|) \\
&+ \sum_{k<l} P_\lambda(\|B_{kl}\|) + \sum_{i<j} U_{ij}^T(A_{ij} - (X_i - X_j)) + \frac{\delta}{2}\sum_{i<j}\|A_{ij} - (X_i - X_j)\|_2^2 \\
&+ \sum_{k<l} V_{kl}^T(B_{kl} - (X^k - X^l)) + \frac{\delta}{2}\sum_{k<l}\|B_{kl} - (X^k - X^l)\|_2^2
\end{aligned} \tag{3}
$$

2 ADMM updates

2.1 update X

$$
\begin{aligned}
X^{(k)} = \arg\min_{x} \frac{1}{2}\|Z - X^{(k-1)}\|_F^2 + \gamma\|X_\Omega^{(k-1)}\|_F^2 - \sum_S U_{ij}^T(X_i - X_j) + \frac{\delta}{2}\sum_S \|A_{ij} - (X_i - X_j)\|_2^2 \\
- \sum_K V_{ij}^T(X^k - X^l) + \frac{\delta}{2}\sum_K \|B_{kl} - (X^k - X^l)\|_2^2
\end{aligned} \tag{4}
$$

$$
\begin{aligned}
Vec(X^{(k)}) = \arg\min_{vec(X)} \frac{1}{2}\|Vec(Z) - Vec(X^{(k-1)})\|_F^2 + \gamma\|E_\Omega Vec(X^{(k-1)})\|_F^2 - \sum_S U_s^T E_{ij} Vec(X^{(k-1)}) \\
+ \frac{\delta}{2}\sum_S \|A_{ij} - E_{ij}Vec(X^{(k-1)})\|_2^2 - \sum_N V_n^T E_{kl} Vec(X^{(k-1)}) \\
+ \frac{\delta}{2}\sum_N \|B_{ij} - E_{kl}Vec(X^{(k-1)})\|_2^2
\end{aligned} \tag{5}
$$

$$
\begin{aligned}
f(X) \overset{\text{let}}{=} \frac{1}{2}\|Vec(Z) - Vec(X^{(k-1)})\|_F^2 + \gamma\|E_\Omega Vec(X^{(k-1)})\|_F^2 - \sum_S U_s^T E_{ij} Vec(X^{(k-1)}) \\
+ \frac{\delta}{2}\sum_S \|A_{ij} - E_{ij}Vec(X^{(k-1)})\|_2^2 - \sum_N V_n^T E_{kl} Vec(X^{(k-1)}) \\
+ \frac{\delta}{2}\sum_N \|B_{ij} - E_{kl}Vec(X^{(k-1)})\|_2^2
\end{aligned} \tag{6}
$$

$$
\begin{aligned}
\frac{\partial f(X)}{Vec(X)} = - Vec(Z) + Vec(X) - \gamma E_\Omega^T E_\Omega Vec(X) + \sum_S E_{ij}^T U_s - \delta \sum_{i<j} E_{ij}^T A_{ij} \\
+ \delta \sum_{i<j} E_{ij}^T E_{ij} Vec(X) + \sum_N E_{kl}^T V_n - \delta \sum_{k<l} E_{kl}^T B_{kl} + \delta \sum_{k<l} E_{kl}^T E_{kl} Vec(X)
\end{aligned} \tag{7}
$$

$$
\begin{aligned}
Vec(X) - \gamma E_\Omega^T E_\Omega Vec(X) + \delta \sum_{i<j} E_{ij}^T E_{ij} Vec(X) + \delta \sum_{k<l} E_{kl}^T E_{kl} Vec(X) \\
= Vec(Z) - \sum_S E_{ij}^T U_s + \delta \sum_{i<j} E_{ij}^T A_{ij} - \sum_N E_{kl}^T V_n + \delta \sum_{k<l} E_{kl}^T B_{kl}
\end{aligned} \tag{8}
$$

$$
\begin{aligned}
\left(I - \gamma E_\Omega^T E_\Omega + \delta \sum_{i<j} E_{ij}^T E_{ij} + \delta \sum_{k<l} E_{kl}^T E_{kl} \right) Vec(X) \\
= Vec(Z) - \sum_S E_{ij}^T U_s + \delta \sum_{i<j} E_{ij}^T A_{ij} - \sum_N E_{kl}^T V_n + \delta \sum_{k<l} E_{kl}^T B_{kl}
\end{aligned} \tag{9}
$$

$$Vec(X) = \left(I - \gamma E_\Omega^T E_\Omega + \delta \sum_{i<j} E_{ij}^T E_{ij} + \delta \sum_{k<l} E_{kl}^T E_{kl} \right)^{-1}$$
$$\left(Vec(Z) - \sum_S E_{ij}^T U_s + \delta \sum_{i<j} E_{ij}^T A_{ij} - \sum_N E_{kl}^T V_n + \delta \sum_{k<l} E_{kl}^T B_{kl} \right) \tag{10}$$

2.2 update A_{ij}

$$A_{ij}^{(k)} = \arg\min_A \frac{1}{2} \sum_{i<j} P_\lambda(\|A_{ij}\|) + \sum_{i<j} U^t A_{ij} + \frac{\delta}{2} \sum_{i<j} \|A_{ij} - (X_i - X_j)\|_2^2 \tag{11}$$

2.2.1 if $\|A_{ij}\| \leq \lambda$ and $A_{ij} \neq 0$

$$\frac{1}{2}\lambda \sum_{i<j} \frac{A_{ij}}{\|A_{ij}\|} + \sum_{ij} U_{ij} + \delta \sum (A_{ij} - E_{ij} Vec(X)) = 0 \tag{12}$$

$$\frac{\lambda A_{ij}}{2\|A_{ij}\|} + U_{ij} + \delta(A_{ij} - E_{ij} Vec(X)) = 0 \tag{13}$$

$$\left(1 + \frac{\lambda}{2\|A_{ij}\|\delta}\right) A_{ij} = E_{ij} Vec(X) - \frac{1}{\delta} U_{ij} \tag{14}$$

let $E_{ij} Vec(X) - \frac{1}{\delta} U_{ij} = \gamma_{ij}$

$$\begin{aligned} \|\gamma_{ij}\| &= \left(1 + \frac{\lambda}{2\|A_{ij}\|\delta}\right) \|A_{ij}\| \\ &= \|A_{ij}\| + \frac{\lambda}{2\delta} \end{aligned} \tag{15}$$

$$\|A_{ij}\| = \|\gamma_{ij}\| - \frac{\lambda}{2\delta} \tag{16}$$

back to eq(14)

$$A_{ij} = \left(1 + \frac{\lambda}{2\|A_{ij}\|\delta}\right)^{-1} \left(E_{ij} Vec(X) - \frac{1}{\delta} U_{ij}\right) \tag{17}$$

by eq(16),

$$A_{ij} = \left(1 + \frac{\lambda}{2(\|\gamma_{ij}\| - \frac{\lambda}{2\delta})\delta}\right)^{-1} \left(E_{ij} Vec(X) - \frac{1}{\delta} U_{ij}\right) \tag{18}$$

$$A_{ij} = \left(1 - \frac{\lambda}{2\delta\|\gamma_{ij}\|}\right)\left(E_{ij}Vec(X) - \frac{1}{\delta}U_{ij}\right) \tag{19}$$

$$B_{kl}^{(k)} = \arg\min_{B_{kl}} \sum_{k<l} P_\lambda(\|B_{kl}\|) + V^T B_{kl} + \frac{\delta}{2}\|B_{kl} - (X^k - X^l)\|_2^2 \tag{20}$$

$$U^{(k)} = U^{(k-1)} + \delta\left(A_{ij} - (X_i - X_j)\right) \tag{21}$$

$$V^{(k)} = V^{(k-1)} + \delta\left(B_{kl} - (X^k - X^l)\right) \tag{22}$$