

Appendix for “Multi-Omics Data Integration via Supervised Adaptive Sparse Canonical Correlation Analysis”

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APPENDIX

A. Proof of Theorem 1

In this appendix, we will demonstrate the theoretical convergence of Algorithm 1. The critical point is that the value of the objective function $f(A^k, \{W_i^k, \delta_i^k\}_{i=1}^m)$ strictly decreases with iterations. Accordingly, we will show that updates to A , $\{\delta_i\}_{i=1}^m$, and $\{W_i\}_{i=1}^m$ all result in lower objective function value. Before proving Theorem 1, we first give Lemma 1 [1] and Lemma 2 [2].

Lemma 1. Let $g(x) = x - ax^{\frac{1}{a}}$, where $a \in (0, 1)$. Then for any $x > 0$, $g(x) \leq 1 - a$, and $x = 1$ is the unique maximizer.

Lemma 2. Suppose the compact SVD of matrix $Y = U_Y D_Y V_Y^\top \in \mathbb{R}^{m \times n}$, where $U_Y \in \mathbb{R}^{m \times r}$, $D_Y \in \mathbb{R}^{r \times r}$, $V_Y \in \mathbb{R}^{n \times r}$, and r is rank of matrix Y . Then the optimal X to the problem

$$\max_{X \in \mathcal{S}_{m,n}} \text{tr}(Y^\top X) \quad (\text{A.1})$$

is

$$X = U_Y V_Y^\top, \quad (\text{A.2})$$

where $\mathcal{S}_{m,n}$ is Stiefel manifold of $m \times n$.

For the sake of concise expression, let

$$Q_i(A, W_i) = \sum_{k=1, l=1}^n \|A_{(k,:)} - X_{i(l,:)} W_i\|_F^2 E_{(k,l)},$$

$$\hat{\delta}_i = f_i(A, W_i)^{-q}.$$

The proof of Theorem 1 is given below.

Proof. According to Lemma 2, we know A^{k+1} is an optimal solution of Eq.(12). Therefore, we can derive

$$\sum_{i=1}^m \delta_i^k Q_i(A^{k+1}, W_i^k) \leq \sum_{i=1}^m \delta_i^k Q_i(A^k, W_i^k), \quad (\text{A.3})$$

which means

$$f(A^{k+1}, \{W_i^k, \delta_i^k\}_{i=1}^m) \leq f(A^k, \{W_i^k, \delta_i^k\}_{i=1}^m). \quad (\text{A.4})$$

Based on Algorithm 1, W_i^{k+1} can bring down the objective function. Thus we have

$$Q_i(A^{k+1}, W_i^{k+1}) + \frac{\lambda}{2} \text{tr}(W_i^{k+1 \top} H_i^k W_i^{k+1})$$

$$\leq Q_i(A^{k+1}, W_i^k) + \frac{\lambda}{2} \text{tr}(W_i^k \top H_i^k W_i^k). \quad (\text{A.5})$$

For simplifying expression, let $w_j = W_{i(:,j)}$ in this subsection. Similarly to above, by Lemma 1, let $a = 1/2$, $x = \|w_j^{k+1}\|_2 / \|w_j^k\|_2$, the following inequalities hold

$$\frac{\|w_j^{k+1}\|_2}{\|w_j^k\|_2} - \frac{1}{2} \frac{\|w_j^{k+1}\|_2^2}{\|w_j^k\|_2^2} \leq 1 - \frac{1}{2}. \quad (\text{A.6})$$

Multiplying Eq.(A.6) by $\|w_j^k\|_2$ and summing its over j , we have

$$\sum_{j=1}^d \left(\frac{\|w_j^{k+1}\|_2^2}{\|w_j^k\|_2^2} - \frac{\|w_j^{k+1}\|_2^2}{2\|w_j^k\|_2^2} \right) \leq \sum_{j=1}^d \left(\frac{\|w_j^k\|_2^2}{\|w_j^k\|_2^2} - \frac{\|w_j^k\|_2^2}{2\|w_j^k\|_2^2} \right),$$

which means

$$\lambda \text{tr}(W_i^{k+1 \top} H_i^{k+1} W_i^{k+1}) - \frac{1}{2} \lambda \text{tr}(W_i^{k+1 \top} H_i^k W_i^{k+1})$$

$$\leq \lambda \text{tr}(W_i^k \top H_i^k W_i^k) - \frac{1}{2} \lambda \text{tr}(W_i^k \top H_i^k W_i^k). \quad (\text{A.7})$$

Adding Eq.(A.5) and Eq.(A.7), the following formula will be derived,

$$f_i(A^{k+1}, W_i^{k+1}) \leq f_i(A^{k+1}, W_i^k).$$

Accordingly, the following inequality holds

$$f(A^{k+1}, \{W_i^{k+1}, \delta_i^k\}_{i=1}^m) \leq f(A^{k+1}, \{W_i^k, \delta_i^k\}_{i=1}^m). \quad (\text{A.8})$$

Let $f_i^{k+1} := f_i(A^{k+1}, W_i^{k+1})$. Noting Lemma 1, let $a = 1 - q$, $x = (f_i^{k+1}/f_i^k)^{1-q}$, the following inequalities hold,

$$\frac{(f_i^{k+1})^{1-q}}{(f_i^k)^{1-q}} - \frac{1-q}{2} \frac{f_i^{k+1}}{f_i^k} \leq 1 - \frac{1-q}{2} \quad (\text{A.9})$$

for $i = 1, 2, \dots, m$. Multiplying Eq.(A.9) by $(f_i^k)^{1-q}$, we have following inequalities simultaneously

$$\frac{f_i^{k+1}}{(f_i^{k+1})^q} - \frac{1-q}{2} \frac{f_i^{k+1}}{(f_i^k)^q} \leq \frac{f_i^k}{(f_i^k)^q} - \frac{1-q}{2} \frac{f_i^k}{(f_i^k)^q} \quad (\text{A.10})$$

for $i = 1, 2, \dots, m$. Further, we can get

$$\sum_{i=1}^m \left(\hat{\delta}_i^{k+1} f_i^{k+1} - \frac{1-q}{2} \hat{\delta}_i^k f_i^{k+1} \right)$$

$$\leq \sum_{i=1}^m \left(\hat{\delta}_i^k f_i^k - \frac{1-q}{2} \hat{\delta}_i^k f_i^k \right). \quad (\text{A.11})$$

Combining Eq.(A.4) and Eq.(A.8), we arrive at

$$f\left(A^{k+1}, \{W_i^{k+1}, \delta_i^k\}_{i=1}^m\right) \leq f\left(A^k, \{W_i^k, \delta_i^k\}_{i=1}^m\right) \quad (\text{A.12})$$

and

$$f\left(A^{k+1}, \{W_i^{k+1}, \hat{\delta}_i^k\}_{i=1}^m\right) \leq f\left(A^k, \{W_i^k, \hat{\delta}_i^k\}_{i=1}^m\right). \quad (\text{A.13})$$

Combining Eq.(A.11) and Eq.(A.13), we can get

$$\sum_{i=1}^m \hat{\delta}_i^{k+1} f_i^{k+1} \leq \sum_{i=1}^m \hat{\delta}_i^k f_i^k. \quad (\text{A.14})$$

Since $\hat{\delta}_i^{k+1} \geq \hat{\delta}_i^k$ for any $i = 1, 2, \dots, m$, according to Eq.(A.14) the following inequality holds,

$$f\left(A^{k+1}, \{W_i^k, \delta_i^{k+1}\}_{i=1}^m\right) \leq f\left(A^k, \{W_i^k, \delta_i^k\}_{i=1}^m\right). \quad (\text{A.15})$$

Based on Eq.(A.15) and Eq.(A.8), we can easily derive the following inequality

$$f\left(A^{k+1}, \{W_i^{k+1}, \delta_i^{k+1}\}_{i=1}^m\right) \leq f\left(A^k, \{W_i^k, \delta_i^k\}_{i=1}^m\right).$$

Consequently, the sequence $\{f(A^k, \{W_i^k, \delta_i^k\}_{i=1}^m)\}$ generated by Algorithm 1 converges since $f(A, \{W_i, \delta_i\}_{i=1}^m)$ has a lower bound. \square

B. Proof of Theorem 2

To prove Theorem 2, we first introduce the following Lemma.

Lemma 3. For any $0 < \epsilon < 1$, with probability $1 - \epsilon$, the following inequality holds,

$$|\mathcal{L} - \hat{\mathcal{L}}| \leq \frac{8Mm^2}{\sqrt{n}} + 2M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}, \quad (\text{A.16})$$

where \mathcal{L} and $\hat{\mathcal{L}}$ are defined in Eq.(25) and Eq.(26), respectively.

Proof. Inspired by [3], for any samples $S = \{x_1, x_2, \dots, x_n\}$, let S' be samples different from S by only one instance x'_r . The empirical risk of the hypothesis function on S' is denoted as $\hat{\mathcal{L}}'$. We have

$$\begin{aligned} & \left| \sup_{h \in \mathcal{H}} |\mathcal{L} - \hat{\mathcal{L}}| - \sup_{h \in \mathcal{H}} |\mathcal{L} - \hat{\mathcal{L}}'| \right| \\ & \leq \sup_{h \in \mathcal{H}} |\hat{\mathcal{L}} - \hat{\mathcal{L}}'| \\ & \leq \sup_{h \in \mathcal{H}} \frac{1}{n^2} \left(\sum_{i=1}^m (|h_i(x_r, x_r)| + |h_i(x'_r, x'_r)|) \right. \\ & \quad \left. + \sum_{i=1}^m \sum_{l=1}^n (|h_{i,j}(x_l, x_r)| + |h_{i,j}(x_l, x'_r)|) \right) \\ & \leq \frac{2M}{n^2} (m + m^2 n) \\ & \leq \frac{2M(m^2 + 1)}{n}, \end{aligned}$$

where the last inequality is due to the fact that h is bounded by M and $m < n$. According to the McDiarmid inequality

[4], we have the following inequality holds with probability $1 - \epsilon$,

$$|\mathcal{L} - \hat{\mathcal{L}}| \leq + \mathbb{E}_S \sup_{h \in \mathcal{H}} |\mathcal{L} - \hat{\mathcal{L}}| + 2M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}. \quad (\text{A.17})$$

Then we analyze the upper bound of the expectation term, i.e. $\mathbb{E}_S \sup_{h \in \mathcal{H}} |\mathcal{L} - \hat{\mathcal{L}}|$. First, we have

$$\begin{aligned} & \mathbb{E}_S \sup_{h \in \mathcal{H}} |\mathcal{L} - \hat{\mathcal{L}}| \\ & = \mathbb{E}_S \sup_{h \in \mathcal{H}} \left| \mathcal{L} - \frac{1}{n^2} \sum_{i=1}^m \sum_{l=1}^n h_i(x_l, x_l) - \frac{1}{n^2} \sum_{i=1}^m \sum_{j=1}^n \sum_{s=1}^n h_{i,j}(x_l, x_s) \right| \\ & \leq \mathbb{E}_S \sup_{h \in \mathcal{H}} \left| \mathcal{L}_1 - \frac{1}{n^2} \sum_{i=1}^m \sum_{l=1}^n h_i(x_l, x_l) \right| \\ & \quad + \mathbb{E}_S \sup_{h \in \mathcal{H}} \left| \mathcal{L}_2 - \frac{1}{n^2} \sum_{i=1}^m \sum_{j=1}^n \sum_{s=1}^n h_{i,j}(x_l, x_s) \right|, \end{aligned}$$

where $\mathcal{L}_1 = \sum_{i=1}^m \mathbb{E}_x h_i(x, x)$ and $\mathcal{L}_2 = \sum_{i=1}^m \sum_{j=1}^n \mathbb{E}_{x,y} h_{i,j}(x, y)$. Let $\sigma_1, \sigma_2, \dots, \sigma_n$ be i.i.d. Rademacher random variables taking values in $\{-1, 1\}$ with equal probability and $\bar{S} = \{\bar{x}_1, \bar{x}_2, \dots, \bar{x}_n\}$ be an independent copy of S . Then the first term can be bounded by

$$\begin{aligned} & \mathbb{E}_S \sup_{h \in \mathcal{H}} \left| \mathcal{L}_1 - \frac{1}{n^2} \sum_{i=1}^m \sum_{l=1}^n h_i(x_l, x_l) \right| \\ & \leq \mathbb{E}_{S, \bar{S}} \sup_{h \in \mathcal{H}} \left| \frac{1}{n^2} \sum_{i=1}^m \sum_{l=1}^n (h_i(x_l, x_l) - h_i(\bar{x}_l, \bar{x}_l)) \right| \\ & = \mathbb{E}_{S, \bar{S}, \sigma} \sup_{h \in \mathcal{H}} \left| \frac{1}{n^2} \sum_{i=1}^m \sum_{l=1}^n \sigma_l (h_i(x_l, x_l) - h_i(\bar{x}_l, \bar{x}_l)) \right| \\ & = 2 \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \frac{1}{n^2} \sum_{i=1}^m \sum_{l=1}^n \sigma_l h_i(x_l, x_l) \right| \\ & \leq \frac{2m}{n^2} \max_i \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \sum_{l=1}^n \sigma_l h_i(x_l, x_l) \right|. \end{aligned}$$

The second term can be bounded by

$$\begin{aligned} & \mathbb{E}_S \sup_{h \in \mathcal{H}} \left| \mathcal{L}_2 - \frac{1}{n^2} \sum_{i=1}^m \sum_{j=1}^n \sum_{s=1}^n h_{i,j}(x_l, x_s) \right| \\ & = \mathbb{E}_{S, \bar{S}} \sup_{h \in \mathcal{H}} \left| \frac{1}{n^2} \sum_{i=1}^m \sum_{j=1}^n \sum_{s=1}^n (h_{i,j}(x_l, x_s) - h_{i,j}(\bar{x}_l, \bar{x}_s)) \right| \\ & \leq \mathbb{E}_{S, \bar{S}} \sup_{h \in \mathcal{H}} \left| \frac{1}{n(n-1)} \sum_{i=1}^m \sum_{j=1}^n \sum_{l \neq s} (h_{i,j}(x_l, x_s) - h_{i,j}(\bar{x}_l, \bar{x}_s)) \right| \end{aligned}$$

$$\begin{aligned}
& + \mathbb{E}_{S, \bar{S}} \sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^m \sum_{l=1}^n (h_{i,j}(x_l, x_l) - h_{i,j}(\bar{x}_l, \bar{x}_l)) \right| \\
& \leq \mathbb{E}_{S, \bar{S}} \sup_{h \in \mathcal{H}} \left| \frac{1}{[n/2]} \sum_{i=1}^m \sum_{l=1}^{[n/2]} \left(h_{i,j}(x_l, x_{l+[n/2]}) - h_{i,j}(\bar{x}_l, \bar{x}_{l+[n/2]}) \right) \right| \\
& + \mathbb{E}_{S, \bar{S}} \sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^m \sum_{l=1}^n (h_{i,j}(x_l, x_l) - h_{i,j}(\bar{x}_l, \bar{x}_l)) \right| \\
& = 2 \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \frac{1}{[n/2]} \sum_{i=1}^m \sum_{l=1}^{[n/2]} \sigma h_{i,j}(x_l, x_{l+[n/2]}) \right| \\
& + 2 \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^m \sum_{l=1}^n \sigma h_{i,j}(x_l, x_l) \right| \\
& \leq \frac{2m^2}{[n/2]} \max_{i,j} \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \sum_{l=1}^{[n/2]} \sigma h_{i,j}(x_l, x_{l+[n/2]}) \right| \\
& + \frac{2m^2}{n} \max_{i,j} \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \sum_{l=1}^n \sigma h_{i,j}(x_l, x_l) \right|,
\end{aligned}$$

where the second inequality is obtained by the Lemma A.1 in [5]. Combining the above results, according to the Khintchine-Kahane inequality [6], we have

$$\begin{aligned}
& \mathbb{E}_S \sup_{h \in \mathcal{H}} |\mathcal{L} - \hat{\mathcal{L}}| \\
& \leq \frac{2m}{n^2} \max_i \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \sum_{l=1}^n \sigma_l h_i(x_l, x_l) \right| \\
& + \frac{2m^2}{[n/2]} \max_{i,j} \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \sum_{l=1}^{[n/2]} \sigma h_{i,j}(x_l, x_{l+[n/2]}) \right| \\
& + \frac{2m^2}{n} \max_{i,j} \mathbb{E}_{S, \sigma} \sup_{h \in \mathcal{H}} \left| \sum_{l=1}^n \sigma h_{i,j}(x_l, x_l) \right| \\
& \leq \frac{2m}{n^2} \max_i \mathbb{E}_S \sup_{h \in \mathcal{H}} \left(\sum_{l=1}^n h_i(x_l, x_l)^2 \right)^{\frac{1}{2}} \\
& + \frac{2m^2}{[n/2]} \max_{i,j} \mathbb{E}_S \sup_{h \in \mathcal{H}} \left(\sum_{l=1}^{[n/2]} h_{i,j}(x_l, x_{l+[n/2]})^2 \right)^{\frac{1}{2}} \\
& + \frac{2m^2}{n} \max_{i,j} \mathbb{E}_S \sup_{h \in \mathcal{H}} \left(\sum_{l=1}^n h_{i,j}(x_l, x_l)^2 \right)^{\frac{1}{2}} \\
& \leq \frac{2Mm}{n\sqrt{n}} + \frac{2Mm^2}{\sqrt{[n/2]}} + \frac{2Mm^2}{\sqrt{n}} \leq \frac{8Mm^2}{\sqrt{n}}.
\end{aligned}$$

Incorporating this bound into Eq.(A.17), we have the following inequality holds with probability $1 - \epsilon$,

$$|\mathcal{L} - \hat{\mathcal{L}}| \leq \frac{8Mm^2}{\sqrt{n}} + 2M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}. \quad (\text{A.18})$$

□

The proof of Theorem 2 is given below.

Proof. Let $\hat{\mathcal{L}}^*$ and $\hat{\mathcal{L}}_f^*$ are optimal empirical risk for the models corresponding adaptive and fixed weights, and the expectation risk are \mathcal{L}^* and \mathcal{L}_f^* , respectively. According to Lemma 3, with probability $1 - \epsilon$, the following inequalities holds,

$$\mathcal{L}^* - \hat{\mathcal{L}}^* \leq \frac{8Mm^2}{\sqrt{n}} + 2M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}, \quad (\text{A.19a})$$

$$\hat{\mathcal{L}}_f^* - \mathcal{L}_f^* \leq \frac{8Mm^2}{\sqrt{n}} + 2M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}. \quad (\text{A.19b})$$

Combing Eq.(A.19a) and Eq.(A.19b), the following inequality holds with probability $1 - \epsilon$,

$$\mathcal{L}^* + \hat{\mathcal{L}}_f^* - \hat{\mathcal{L}}^* \leq \mathcal{L}_f^* + \frac{16Mm^2}{\sqrt{n}} + 4M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}. \quad (\text{A.20})$$

Notice that since the δ_i in \mathcal{L}_f^* is fixed, yet the δ_i in \mathcal{L}^* is required to be optimized, as thus $\hat{\mathcal{L}}_f^* - \hat{\mathcal{L}}^* \geq 0$. Accordingly, with at least probability $1 - \epsilon$, we have

$$\mathcal{L}^* \leq \mathcal{L}_f^* + \frac{16Mm^2}{\sqrt{n}} + 4M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}. \quad (\text{A.21})$$

□

C. The proof of Corollary 1

Notably, Since the definition Eq.(10) of the weights shows that δ_i cannot be taken to 1 or 0 for all i , Corollary 1 needs to be proved in the sense of a limit. This part of the proof relies heavily on the inequality between two sequences preserved in the limit, i.e.,

Lemma 4. *Let both $\{a_n\}$ and $\{b_n\}$ be convergent sequences. If there exists a positive integer N such that $a_n < b_n$ when $n > N$, then $\lim_{n \rightarrow \infty} a_n \leq \lim_{n \rightarrow \infty} b_n$.*

The proof of Corollary 1 is given below.

Proof. Without loss of generality, let the weights be $\{\delta_i = 1 - \sum_{j \neq i} \delta_j, \delta_j = 1/n | j \neq i\}$, then the $\{\hat{\mathcal{L}}_{i(n)}^*\}$ can be viewed a sequence about n . According to subsection B, we have $\hat{\mathcal{L}}_{i(n)}^* \geq \hat{\mathcal{L}}^*$ for any $n \in \mathbb{N}$. Clearly, $\hat{\mathcal{L}}_{i(n)}^*$ converges to $\hat{\mathcal{L}}_i^*$ when n tends to infinity. Thus by Lemma 4, it follows that $\hat{\mathcal{L}}_i^* \geq \hat{\mathcal{L}}^*$ holds. Furthermore, similar to Eq.(A.21), we can get the following inequality holds with at least probability $1 - \epsilon$,

$$\mathcal{L}^* \leq \mathcal{L}_i^* + \frac{16Mm^2}{\sqrt{n}} + 4M(m^2 + 1) \sqrt{\frac{\log \frac{2}{\epsilon}}{2n}}. \quad (\text{A.22})$$

□

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