

A Proof of Theorem 1

Proof. It is easy to see that by the end of the first iteration of Algorithm 1, $\tilde{\psi}_1$ and ψ_1 lie in the span of $\{\mathbf{b}_i\}_{i=1}^r$, while $\tilde{\phi}_1$ and ϕ_1 lie in the span of $\{\mathbf{a}_i\}_{i=1}^r$. And therefore they remain in these spaces for all $t \geq 1$.

Let us first focus on ϕ_t . For $t \geq 2$, we observe that

$$\phi_t = \mathbf{T}\psi_{t-1} / \|\tilde{\phi}_t\| = \mathbf{T}\mathbf{T}^\top \phi_{t-2} / (\|\tilde{\phi}_t\| \cdot \|\tilde{\psi}_{t-1}\|).$$

Since $\|\phi_{t-2}\| = \|\phi_t\| = 1$, it is equivalent to using the following updates:

$$\phi_t \leftarrow \mathbf{T}\mathbf{T}^\top \phi_{t-2}, \quad \phi_t \leftarrow \phi_t / \|\phi_t\|.$$

This indicates that, Algorithm 1 runs the standard power iterations on $\mathbf{T}\mathbf{T}^\top$ to generate the $\{\phi_t\}_{t \geq 1}$ sequence for every two steps.

(i) For $t = 2, 4, \dots$, we have $\phi_t = \frac{(\mathbf{T}\mathbf{T}^\top)^{\frac{t}{2}} \phi_0}{\|(\mathbf{T}\mathbf{T}^\top)^{\frac{t}{2}} \phi_0\|}$. Let $\mathbf{M} = \mathbf{T}\mathbf{T}^\top$, whose nonzero eigenvalues are $\rho_1^2 \geq \rho_2^2 \geq \dots \geq \rho_r^2 > 0$, with corresponding eigenvectors $\mathbf{a}_1, \dots, \mathbf{a}_r$. Then, for $i = 1, \dots, r$,

$$\begin{aligned} (\mathbf{a}_i^\top \phi_t)^2 &= \frac{(\mathbf{a}_i^\top \mathbf{M}^{\frac{t}{2}} \phi_0)^2}{\|\mathbf{M}^{\frac{t}{2}} \phi_0\|^2} = \frac{(\mathbf{a}_i^\top \mathbf{M}^{\frac{t}{2}} \phi_0)^2}{\phi_0^\top \mathbf{M}^t \phi_0} = \frac{(\rho_i^t \mathbf{a}_i^\top \phi_0)^2}{\sum_{j=1}^r \rho_j^{2t} (\mathbf{a}_j^\top \phi_0)^2} = \frac{(\mathbf{a}_i^\top \phi_0)^2}{\sum_{j=1}^r \left(\frac{\rho_j^2}{\rho_i^2}\right)^t (\mathbf{a}_j^\top \phi_0)^2} \\ &\leq \frac{(\mathbf{a}_i^\top \phi_0)^2}{\left(\frac{\rho_1^2}{\rho_i^2}\right)^t (\mathbf{a}_1^\top \phi_0)^2} = \frac{(\mathbf{a}_i^\top \phi_0)^2}{(\mathbf{a}_1^\top \phi_0)^2} \left(\frac{\rho_i^2}{\rho_1^2}\right)^t = \frac{(\mathbf{a}_i^\top \phi_0)^2}{(\mathbf{a}_1^\top \phi_0)^2} \left(1 - \frac{\rho_1^2 - \rho_i^2}{\rho_1^2}\right)^t \\ &\leq \frac{(\mathbf{a}_i^\top \phi_0)^2}{(\mathbf{a}_1^\top \phi_0)^2} \exp\left(-\frac{\rho_1^2 - \rho_i^2}{\rho_1^2} t\right). \end{aligned}$$

(ii) For $t = 1, 3, \dots$, we have $\phi_t = \frac{(\mathbf{T}\mathbf{T}^\top)^{\frac{t-1}{2}} \mathbf{T}\psi_0}{\|(\mathbf{T}\mathbf{T}^\top)^{\frac{t-1}{2}} \mathbf{T}\psi_0\|}$. Let $\mathbf{N} = \mathbf{T}^\top \mathbf{T}$, whose nonzero eigenvalues are $\rho_1^2 \geq \rho_2^2 \geq \dots \geq \rho_r^2 > 0$, with corresponding eigenvectors $\mathbf{b}_1, \dots, \mathbf{b}_r$. Then, for $i = 1, \dots, r$,

$$\begin{aligned} (\mathbf{a}_i^\top \phi_t)^2 &= \frac{(\mathbf{a}_i^\top (\mathbf{T}\mathbf{T}^\top)^{\frac{t-1}{2}} \mathbf{T}\psi_0)^2}{\|(\mathbf{T}\mathbf{T}^\top)^{\frac{t-1}{2}} \mathbf{T}\psi_0\|^2} = \frac{((\mathbf{T}^\top \mathbf{a}_i)^\top \mathbf{N}^{\frac{t-1}{2}} \psi_0)^2}{\psi_0^\top \mathbf{N}^t \psi_0} = \frac{(\rho_i^t \mathbf{b}_i^\top \psi_0)^2}{\sum_{j=1}^r \rho_j^{2t} (\mathbf{b}_j^\top \psi_0)^2} \\ &\leq \frac{(\mathbf{b}_i^\top \psi_0)^2}{(\mathbf{b}_1^\top \psi_0)^2} \exp\left(-\frac{\rho_1^2 - \rho_i^2}{\rho_1^2} t\right). \end{aligned}$$

Given $\delta \in (0, 1)$, define $S(\delta) = \{i : \rho_i^2 > (1 - \delta)\rho_1^2\}$. For $\delta_1, \delta_2 \in (0, 1)$, define

$$T(\delta_1, \delta_2) := \lceil \frac{1}{\delta_1} \log\left(\frac{1}{\mu\delta_2}\right) \rceil.$$

For all $i \notin S(\delta_1)$, when $t > T(\delta_1, \delta_2)$, it holds that $(\mathbf{a}_i^\top \phi_t)^2 \leq \delta_2 (\mathbf{a}_i^\top \phi_0)^2$ if t is even, and $(\mathbf{a}_i^\top \phi_t)^2 \leq \delta_2 (\mathbf{b}_i^\top \psi_0)^2$ if t is odd. In both cases, we have $\sum_{i \in S(\delta_1)} (\mathbf{a}_i^\top \phi_t)^2 \geq 1 - \delta_2$.

When there exists a positive singular value gap, i.e., $\rho_1 - \rho_2 > 0$, set $\delta_1 = (\rho_1^2 - \rho_2^2)/\rho_1^2$ and thus $S(\delta_1) = 1$. Furthermore, set $\delta_2 = \eta$ and we obtain $(\mathbf{a}_1^\top \phi_t)^2 \geq 1 - \eta$.

The proof for ψ_t is completely analogous. To obtain the bound on the objective, we have

$$\begin{aligned}
\mathbf{u}_t^\top \Sigma_{xy} \mathbf{v}_t &= \phi_t^\top \mathbf{T} \psi_t = \rho_1 (\phi_t^\top \mathbf{a}_1) (\psi_t^\top \mathbf{b}_1) + \sum_{i=2}^r \rho_i (\phi_t^\top \mathbf{a}_i) (\psi_t^\top \mathbf{b}_i) \\
&\geq \rho_1 (\phi_t^\top \mathbf{a}_1) (\psi_t^\top \mathbf{b}_1) - \rho_1 \sum_{i=2}^r \left| \phi_t^\top \mathbf{a}_i \right| \left| \psi_t^\top \mathbf{b}_i \right| \\
&\geq \rho_1 (1 - \eta) - \rho_1 \sqrt{\sum_{i=2}^r \left(\phi_t^\top \mathbf{a}_i \right)^2} \sqrt{\sum_{i=2}^r \left(\psi_t^\top \mathbf{b}_i \right)^2} \\
&\geq \rho_1 (1 - \eta) - \rho_1 \eta = \rho_1 (1 - 2\eta),
\end{aligned}$$

where we have used the Cauchy-Schwarz inequality in the second inequality. \square

B Proof of Theorem 2

From now on, we distinguish the iterates of our stochastic algorithm (Algorithm 2) from the iterates of the exact power iterations (Algorithm 1) and denote the latter with asterisks, i.e., $\tilde{\mathbf{u}}_t^*$ and $\tilde{\mathbf{v}}_t^*$ for the unnormalized iterates and \mathbf{u}_t^* and \mathbf{v}_t^* for the normalized iterates. We denote the exact optimum of $f_t(\mathbf{u})$ and $g_t(\mathbf{v})$ by $\bar{\mathbf{u}}_t$ and $\bar{\mathbf{v}}_t$ respectively.

The following lemma bounds the distance between the iterates of inexact and exact power iterations.

Lemma 6. Assume that Algorithm 1 and Algorithm 2 start with the same initialization, i.e., $\tilde{\mathbf{u}}_0 = \tilde{\mathbf{u}}_0^*$ and $\tilde{\mathbf{v}}_0 = \tilde{\mathbf{v}}_0^*$. Then, for $t \geq 1$, the unnormalized iterates of Algorithm 2 satisfy

$$\max \left(\left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \right\|, \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t - \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t^* \right\| \right) \leq \tilde{S}_t,$$

where

$$\tilde{S}_t := \sqrt{2\epsilon} \frac{(2\rho_1/\rho_r)^t - 1}{(2\rho_1/\rho_r) - 1}.$$

Furthermore, for $t \geq 1$, the normalized iterates of Algorithm 2 satisfy

$$\max \left(\left\| \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t - \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t^* \right\|, \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t - \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t^* \right\| \right) \leq S_t := \frac{2\tilde{S}_t}{\rho_r}.$$

Proof. We focus on the $\{\tilde{\mathbf{u}}_t\}_{t \geq 0}$ and $\{\mathbf{u}_t\}_{t \geq 0}$ sequences below; the proof for $\{\tilde{\mathbf{v}}_t\}_{t \geq 0}$ and $\{\mathbf{v}_t\}_{t \geq 0}$ is completely analogous.

We prove the bound for unnormalized iterates by induction. First, the case for $t = 1$ holds trivially. For $t \geq 2$, we can bound the error of the unnormalized iterates using the exact solution to $f_t(\mathbf{u})$:

$$\left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \right\| \leq \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \right\| + \left\| \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \right\|. \quad (14)$$

For the first term of (14), notice $f_t(\mathbf{u})$ is a quadratic function with minimum achieved at $\bar{\mathbf{u}}_t = \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_{t-1}$. For the approximate solution $\tilde{\mathbf{u}}_t$, we have

$$f_t(\tilde{\mathbf{u}}_t) - f_t(\bar{\mathbf{u}}_t) = \frac{1}{2} (\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t)^\top \Sigma_{xx} (\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t) = \frac{1}{2} \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \right\|^2 \leq \epsilon.$$

It then follows that $\left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \right\| \leq \sqrt{2\epsilon}$.

The second term of (14) is concerned with the error due to inexact target in the least squares problem $f_t(\mathbf{u})$ as \mathbf{v}_{t-1} is different from \mathbf{v}_{t-1}^* . We can bound it as

$$\begin{aligned}
\left\| \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \right\| &= \left\| \Sigma_{xx}^{\frac{1}{2}} \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_{t-1} - \Sigma_{xx}^{\frac{1}{2}} \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_{t-1}^* \right\| \\
&= \left\| \left(\Sigma_{xx}^{-\frac{1}{2}} \Sigma_{xy} \Sigma_{yy}^{-\frac{1}{2}} \right) \left(\Sigma_{yy}^{\frac{1}{2}} (\mathbf{v}_{t-1} - \mathbf{v}_{t-1}^*) \right) \right\| \\
&\leq \|\mathbf{T}\| \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} - \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1}^* \right\| = \rho_1 \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} - \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1}^* \right\|. \quad (15)
\end{aligned}$$

In view of the update rule of our algorithm and the triangle inequality, we have

$$\begin{aligned}
& \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} - \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1}^* \right\| \\
& \leq \left\| \frac{\Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} - \frac{\Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\|} \right\| + \left\| \frac{\Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} - \frac{\Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^*}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\|} \right\| \\
& = \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\| \left| \frac{1}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} - \frac{1}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\|} \right| + \frac{1}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} - \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\| \\
& = \frac{1}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} \left| \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\| - \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\| \right| + \frac{1}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} - \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\| \\
& \leq \frac{2}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|} \left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} - \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\| \leq \frac{2\tilde{S}_{t-1}}{\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1} \right\|}. \tag{16}
\end{aligned}$$

We now bound $\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\|$ from below. Since $t \geq 2$, we have

$$\Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* = \Sigma_{yy}^{\frac{1}{2}} \Sigma_{yy}^{-1} \Sigma_{xy}^\top \mathbf{u}_{t-2}^* = \left(\Sigma_{yy}^{-\frac{1}{2}} \Sigma_{xy}^\top \Sigma_{xx}^{-\frac{1}{2}} \right) \left(\Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_{t-2}^* \right) = \mathbf{T}^\top \left(\Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_{t-2}^* \right).$$

Now, $\Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_{t-2}^*$ corresponds to ϕ_{t-2} in Algorithm 1, which has unit length and lies in the span of $\{\mathbf{a}_1, \dots, \mathbf{a}_r\}$, so we have

$$\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_{t-1}^* \right\| = \left\| \mathbf{T}^\top \phi_{t-2} \right\| \geq \rho_r.$$

Combining (14), (15) and (16) gives

$$\begin{aligned}
\left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t - \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \right\| & \leq \sqrt{2\epsilon} + \frac{2\rho_1}{\rho_r} \cdot \tilde{S}_{t-1} = \sqrt{2\epsilon} + \frac{2\rho_1}{\rho_r} \cdot \sqrt{2\epsilon} \frac{(2\rho_1/\rho_r)^{t-1} - 1}{(2\rho_1/\rho_r) - 1} \\
& = \sqrt{2\epsilon} \frac{(2\rho_1/\rho_r)^t - 1}{(2\rho_1/\rho_r) - 1} = \tilde{S}_t.
\end{aligned}$$

The bound for normalized iterates follows from (16). \square

Proof of Theorem 2. We prove the theorem by relating the iterates of inexact power iterations to those of exact power iterations.

Assume the same initialization as in Lemma 6. First observe that

$$\begin{aligned}
(\mathbf{u}_t^\top \Sigma_{xx} \mathbf{u}^*)^2 & = \left((\mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* + (\mathbf{u}_t - \mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* \right)^2 \\
& \geq \left((\mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* \right)^2 + 2 \left((\mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* \right) \left((\mathbf{u}_t - \mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* \right) \\
& \geq \left((\mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* \right)^2 - 2 \left| \left(\Sigma_{xx}^{\frac{1}{2}} (\mathbf{u}_t - \mathbf{u}_t^*) \right)^\top \left(\Sigma_{xx}^{\frac{1}{2}} \mathbf{u}^* \right) \right| \\
& \geq \left((\mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* \right)^2 - 2 \left\| \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t - \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t^* \right\| \tag{17}
\end{aligned}$$

where we have used the fact that $\left\| \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t \right\| = \left\| \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t^* \right\| = \left\| \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}^* \right\| = 1$ and the Cauchy-Schwarz inequality in the last two steps.

Applying Theorem 1 with $T \geq \lceil \frac{\rho_1^2}{\rho_1^2 - \rho_2^2} \log \left(\frac{2}{\mu\eta} \right) \rceil$, we have that $\left((\mathbf{u}_T^*)^\top \Sigma_{xx} \mathbf{u}^* \right)^2 \geq 1 - \eta/2$. On the other hand, in view of Lemma 6, we have for the specified ϵ value in Algorithm 2 that $\left\| \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_T - \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_T^* \right\| \leq S_T = \eta/4$. Plugging these two bounds into (17) gives the desired result.

The proof for \mathbf{v}_T is completely analogous. \square

C SVRG for minimizing $f(\mathbf{u})$

We provide the pseudo-code of SVRG for solving the least squares problem (6) below.

SVRG for $\min_{\mathbf{u}} f(\mathbf{u}) := \frac{1}{N} \sum_{i=1}^N \left(\frac{1}{2} |\mathbf{u}^\top \mathbf{x}_i - \mathbf{v}^\top \mathbf{y}_i|^2 + \frac{\gamma_x}{2} \|\mathbf{u}\|^2 \right)$.

Input: Stepsize ξ .
Initialize $\mathbf{u}_{(0)} \in \mathbb{R}^{d_x}$.
for $j = 1, 2, \dots, M$ **do**
 $\mathbf{w}_0 \leftarrow \mathbf{u}_{(j-1)}$
 Evaluate the batch gradient $\nabla f(\mathbf{w}_0) = \mathbf{X}(\mathbf{X}^\top \mathbf{w}_0 - \mathbf{Y}^\top \mathbf{v})/N + \gamma_x \mathbf{w}_0$
 for $t = 1, 2, \dots, m$ **do**
 Randomly pick i_t from $\{1, \dots, N\}$
 $\mathbf{w}_t \leftarrow \mathbf{w}_{t-1} - \xi \left((\mathbf{x}_{i_t} \mathbf{x}_{i_t}^\top + \gamma_x \mathbf{I})(\mathbf{w}_{t-1} - \mathbf{w}_0) + \nabla f(\mathbf{w}_0) \right)$
 end for
 $\mathbf{u}_{(j)} \leftarrow \mathbf{w}_t$ for randomly chosen $t \in \{1, \dots, m\}$.
end for
Output: $\mathbf{u}_{(M)}$ is the approximate solution.

D Initial suboptimality of warm-starts in Algorithm 2

At time step t , we initialize the least squares problem $f_t(\mathbf{u})$ with the unnormalized iterate $\tilde{\mathbf{u}}_{t-1}$ from the previous time step. We now bound the suboptimality of this initialization. Observe that the minimum of $f_t(\mathbf{u})$ is achieved by $\bar{\mathbf{u}}_t = \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_{t-1}$, and that

$$f_t(\tilde{\mathbf{u}}_{t-1}) - f_t(\bar{\mathbf{u}}_t) = \frac{1}{2} (\tilde{\mathbf{u}}_{t-1} - \bar{\mathbf{u}}_t)^\top \Sigma_{xx} (\tilde{\mathbf{u}}_{t-1} - \bar{\mathbf{u}}_t) = \frac{1}{2} \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_{t-1} - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \right\|^2.$$

Applying the triangle inequality, we have for $t = 1$ that

$$\begin{aligned} \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_0 - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_1 \right\| &\leq \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_0 \right\| + \left\| \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_1 \right\| \leq 1 + \left\| \Sigma_{xx}^{\frac{1}{2}} \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_0 \right\| \\ &= 1 + \left\| \mathbf{T} \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_0 \right\| \leq 1 + \|\mathbf{T}\| \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_0 \right\| = 1 + \rho_1 \leq 2 \end{aligned}$$

where we have used facts that $\left\| \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{u}}_0 \right\| = \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_0 \right\| = 1$ due to the initial normalizations.

And we have for $t \geq 2$ that

$$\begin{aligned} \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_{t-1} - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \right\| &\leq \left\| \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_{t-1} - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_{t-1} \right\| + \left\| \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_{t-1} - \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \right\| \\ &\leq \sqrt{2\epsilon} + \left\| \Sigma_{xx}^{\frac{1}{2}} \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_{t-2} - \Sigma_{xx}^{\frac{1}{2}} \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{v}_{t-1} \right\| \\ &= \sqrt{2\epsilon} + \left\| \mathbf{T} \left(\Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-2} - \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} \right) \right\| \\ &\leq \sqrt{2\epsilon} + \|\mathbf{T}\| \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-2} - \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} \right\| \\ &\leq \sqrt{2\epsilon} + 2\rho_1 \leq \sqrt{2\epsilon} + 2 \end{aligned}$$

where we have used the fact that $\left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-2} \right\| = \left\| \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} \right\| = 1$ in the last inequality.

Therefore, for all $t \geq 1$, the ration between initial suboptimality and required accuracy is

$$\frac{f_t(\tilde{\mathbf{u}}_{t-1}) - f_t(\bar{\mathbf{u}}_t)}{\epsilon} \sim \frac{2}{\epsilon}.$$

E The shift-and-invert preconditioning (SI) algorithm for CCA

Our shift-and-invert preconditioning (SI) meta-algorithm is detailed in Algorithm 3.

Algorithm 3 The shift-and-invert preconditioning meta-algorithm for CCA.

Input: Data matrices \mathbf{X}, \mathbf{Y} , regularization parameters (γ_x, γ_y) , an estimate $\tilde{\Delta}$ for $\Delta = \rho_1 - \rho_2$.

Initialize $\tilde{\mathbf{u}}_0 \in \mathbb{R}^{d_x}, \tilde{\mathbf{v}}_0 \in \mathbb{R}^{d_y}$

$\mathbf{u}_0 \leftarrow \tilde{\mathbf{u}}_0 / \sqrt{\tilde{\mathbf{u}}_0^\top \Sigma_{xx} \tilde{\mathbf{u}}_0}, \quad \mathbf{v}_0 \leftarrow \tilde{\mathbf{v}}_0 / \sqrt{\tilde{\mathbf{v}}_0^\top \Sigma_{yy} \tilde{\mathbf{v}}_0}$

// Phase I: shift-and-invert preconditioning for eigenvectors of \mathbf{M}_λ

$s \leftarrow 0, \quad \lambda_{(0)} \leftarrow 1 + \tilde{\Delta}$

repeat

$s \leftarrow s + 1$

for $t = (s-1)m_1 + 1, \dots, sm_1$ **do**

Optimize the least squares problem

$$\min_{\mathbf{u}, \mathbf{v}} h_t(\mathbf{u}, \mathbf{v}) := \frac{1}{2} [\mathbf{u}^\top \mathbf{v}^\top] \begin{bmatrix} \lambda_{(s-1)} \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda_{(s-1)} \Sigma_{yy} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} - \mathbf{u}^\top \Sigma_{xx} \mathbf{u}_{t-1} - \mathbf{v}^\top \Sigma_{yy} \mathbf{v}_{t-1}$$

and output an approximate solution $(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t)$ satisfying $h_t(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t) \leq \min_{\mathbf{u}, \mathbf{v}} h_t(\mathbf{u}, \mathbf{v}) + \tilde{\epsilon}$.

Normalization: $\begin{bmatrix} \mathbf{u}_t \\ \mathbf{v}_t \end{bmatrix} \leftarrow \sqrt{2} \begin{bmatrix} \tilde{\mathbf{u}}_t \\ \tilde{\mathbf{v}}_t \end{bmatrix} / \sqrt{\tilde{\mathbf{u}}_t^\top \Sigma_{xx} \tilde{\mathbf{u}}_t + \tilde{\mathbf{v}}_t^\top \Sigma_{yy} \tilde{\mathbf{v}}_t}$

end for

Optimize the least squares problem

$$\min_{\mathbf{w}} l_s(\mathbf{w}) := \frac{1}{2} \mathbf{w}^\top \begin{bmatrix} \lambda_{(s-1)} \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda_{(s-1)} \Sigma_{yy} \end{bmatrix} \mathbf{w} - \mathbf{w}^\top \begin{bmatrix} \Sigma_{xx} \mathbf{u}_{sm_1} \\ \Sigma_{yy} \mathbf{v}_{sm_1} \end{bmatrix}$$

and output an approximate solution \mathbf{w}_s satisfying $l_s(\mathbf{w}_s) \leq \min_{\mathbf{w}} l_s(\mathbf{w}) + \tilde{\epsilon}$.

$$\Delta_s \leftarrow \frac{1}{2} \cdot \frac{1}{\frac{1}{2} [\mathbf{u}_{sm_1}^\top \mathbf{v}_{sm_1}^\top] \begin{bmatrix} \Sigma_{xx} & \\ & \Sigma_{yy} \end{bmatrix} \mathbf{w}_s - 2\sqrt{\tilde{\epsilon}/\tilde{\Delta}}}, \quad \lambda_{(s)} \leftarrow \lambda_{(s-1)} - \frac{\Delta_s}{2}$$

until $\Delta_{(s)} \leq \tilde{\Delta}$

$\lambda_{(f)} \leftarrow \lambda_{(s)}$

for $t = sm_1 + 1, sm_1 + 2, \dots, sm_1 + m_2$ **do**

Optimize the least squares problem

$$\min_{\mathbf{u}, \mathbf{v}} h_t(\mathbf{u}, \mathbf{v}) := \frac{1}{2} [\mathbf{u}^\top \mathbf{v}^\top] \begin{bmatrix} \lambda_{(f)} \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda_{(f)} \Sigma_{yy} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} - \mathbf{u}^\top \Sigma_{xx} \mathbf{u}_{t-1} - \mathbf{v}^\top \Sigma_{yy} \mathbf{v}_{t-1}$$

and output an approximate solution $(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t)$ satisfying $h_t(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t) \leq \min_{\mathbf{u}, \mathbf{v}} h_t(\mathbf{u}, \mathbf{v}) + \tilde{\epsilon}$.

Normalization: $\begin{bmatrix} \mathbf{u}_t \\ \mathbf{v}_t \end{bmatrix} \leftarrow \sqrt{2} \begin{bmatrix} \tilde{\mathbf{u}}_t \\ \tilde{\mathbf{v}}_t \end{bmatrix} / \sqrt{\tilde{\mathbf{u}}_t^\top \Sigma_{xx} \tilde{\mathbf{u}}_t + \tilde{\mathbf{v}}_t^\top \Sigma_{yy} \tilde{\mathbf{v}}_t}$

end for

// Phase II: Final normalization

$$T \leftarrow sm_1 + m_2, \quad \hat{\mathbf{u}} \leftarrow \mathbf{u}_T / \sqrt{\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}_T}, \quad \hat{\mathbf{v}} \leftarrow \mathbf{v}_T / \sqrt{\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}_T}$$

Output: $(\hat{\mathbf{u}}, \hat{\mathbf{v}})$ is the approximate solution to CCA.

F Proof of Theorem 4

The proof of Theorem 4 closely follows that of [16, Theorem 4.2]. And we will need a few lemmas on the convergence of inexact power iterations.

F.1 Auxiliary lemmas

Define the condition number of \mathbf{M}_λ as

$$\kappa_\lambda := \frac{\sigma_1(\mathbf{M}_\lambda)}{\sigma_d(\mathbf{M}_\lambda)} = \frac{\frac{1}{\lambda - \rho_1}}{\frac{1}{\lambda + \rho_1}} = \frac{\lambda + \rho_1}{\lambda - \rho_1},$$

and the inverse relative spectral gap of \mathbf{M}_λ as

$$\delta_\lambda := \frac{\sigma_1(\mathbf{M}_\lambda)}{\sigma_1(\mathbf{M}_\lambda) - \sigma_2(\mathbf{M}_\lambda)} = \frac{\frac{1}{\lambda - \rho_1}}{\frac{1}{\lambda - \rho_1} - \frac{1}{\lambda - \rho_2}} = \frac{\lambda - \rho_2}{\rho_1 - \rho_2}.$$

The first lemma states the convergence of exact power iterations, paralleling [16, Theorem A.1].

Lemma 7 (Convergence of exact power iterations). Fix $\alpha > 0$. For the exact power iterations on \mathbf{M}_λ where

$$\begin{aligned} \begin{bmatrix} \tilde{\mathbf{u}}_t^* \\ \tilde{\mathbf{v}}_t^* \end{bmatrix} &\leftarrow \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix}^{-1} \begin{bmatrix} \Sigma_{xx} & \\ & \Sigma_{yy} \end{bmatrix} \begin{bmatrix} \mathbf{u}_{t-1}^* \\ \mathbf{v}_{t-1}^* \end{bmatrix}, \\ \begin{bmatrix} \mathbf{u}_t^* \\ \mathbf{v}_t^* \end{bmatrix} &\leftarrow \sqrt{2} \begin{bmatrix} \tilde{\mathbf{u}}_t^* \\ \tilde{\mathbf{v}}_t^* \end{bmatrix} \Big/ \sqrt{(\tilde{\mathbf{u}}_t^*)^\top \Sigma_{xx} \tilde{\mathbf{u}}_t^* + (\tilde{\mathbf{v}}_t^*)^\top \Sigma_{yy} \tilde{\mathbf{v}}_t^*}, \quad \text{for } t = 1, \dots, m, \end{aligned}$$

and $\mu' := \frac{1}{4} ((\mathbf{u}_0^*)^\top \Sigma_{xx} \mathbf{u}^* + (\mathbf{v}_0^*)^\top \Sigma_{yy} \mathbf{v}^*)^2 > 0$, we have

- (crude regime)

$$\frac{1}{2} \left[(\mathbf{u}_t^*)^\top \Sigma_{xx}^{\frac{1}{2}}, (\mathbf{v}_t^*)^\top \Sigma_{yy}^{\frac{1}{2}} \right] \mathbf{M}_\lambda \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t^* \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t^* \end{bmatrix} \geq (1 - \alpha) \cdot \sigma_1(\mathbf{M}_\lambda)$$

for $t \geq \lceil \frac{1}{\alpha} \log \left(\frac{2}{\mu' \alpha} \right) \rceil$,

- (accurate regime)

$$\frac{1}{4} ((\mathbf{u}_t^*)^\top \Sigma_{xx} \mathbf{u}^* + (\mathbf{v}_t^*)^\top \Sigma_{yy} \mathbf{v}^*)^2 \geq 1 - \alpha$$

for $t \geq \lceil \frac{\delta_\lambda}{2} \log \left(\frac{1}{\mu' \alpha} \right) \rceil$.

The second lemma bounds the distances between the iterates of inexact and exact power iterations, paralleling [16, Lemma 4.1]. Recall that the $(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t)$ in Algorithm 3 satisfies $h_t(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t) \leq \min_{\mathbf{u}, \mathbf{v}} h_t(\mathbf{u}, \mathbf{v}) + \tilde{\epsilon}$. Let $(\bar{\mathbf{u}}_t, \bar{\mathbf{v}}_t)$ be the exact minimum of h_t . Then we have

$$\begin{aligned} &h_t(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t) - h_t(\bar{\mathbf{u}}_t, \bar{\mathbf{v}}_t) \\ &= \frac{1}{2} [(\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t)^\top \quad (\tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t)^\top] \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t \\ \tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t \end{bmatrix} \\ &= \frac{1}{2} [(\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t)^\top \quad (\tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t)^\top] \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t \\ \tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t \end{bmatrix} \\ &= \frac{1}{2} [(\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t)^\top \Sigma_{xx}^{\frac{1}{2}} \quad (\tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t)^\top \Sigma_{yy}^{\frac{1}{2}}] \begin{bmatrix} \lambda \mathbf{I} & -\mathbf{T} \\ -\mathbf{T}^\top & \lambda \mathbf{I} \end{bmatrix} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} (\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t) \\ \Sigma_{yy}^{\frac{1}{2}} (\tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t) \end{bmatrix} \\ &= \frac{1}{2} [(\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t)^\top \Sigma_{xx}^{\frac{1}{2}} \quad (\tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t)^\top \Sigma_{yy}^{\frac{1}{2}}] \mathbf{M}_\lambda^{-1} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} (\tilde{\mathbf{u}}_t - \bar{\mathbf{u}}_t) \\ \Sigma_{yy}^{\frac{1}{2}} (\tilde{\mathbf{v}}_t - \bar{\mathbf{v}}_t) \end{bmatrix} \leq \tilde{\epsilon}. \end{aligned} \tag{18}$$

Lemma 8 (Power iterations with inexact matrix-vector multiplications). Consider the inexact power iterations on \mathbf{M}_λ where

$$\begin{aligned} &(\tilde{\mathbf{u}}_t, \tilde{\mathbf{v}}_t) \text{ satisfies } (18), \\ &\begin{bmatrix} \mathbf{u}_t \\ \mathbf{v}_t \end{bmatrix} \leftarrow \sqrt{2} \begin{bmatrix} \tilde{\mathbf{u}}_t \\ \tilde{\mathbf{v}}_t \end{bmatrix} \Big/ \sqrt{\tilde{\mathbf{u}}_t^\top \Sigma_{xx} \tilde{\mathbf{u}}_t + \tilde{\mathbf{v}}_t^\top \Sigma_{yy} \tilde{\mathbf{v}}_t}, \quad \text{for } t = 1, \dots, m. \end{aligned}$$

Compare these iterates with those of the exact power iterations described in Lemma 7 using the same initialization $\tilde{\mathbf{u}}_0 = \tilde{\mathbf{u}}_0^*$, $\tilde{\mathbf{v}}_0 = \tilde{\mathbf{v}}_0^*$. Then, for $t \geq 0$, the unnormalized iterates satisfy

$$\left\| \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t \end{bmatrix} - \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t^* \end{bmatrix} \right\| \leq \tilde{R}_t$$

where

$$\tilde{R}_t := \sqrt{\sigma_1(\mathbf{M}_\lambda)} \cdot \tilde{\epsilon} \cdot \frac{(2\kappa_\lambda)^t - 1}{2\kappa_\lambda - 1},$$

while the normalized iterates satisfy

$$\left\| \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t \end{bmatrix} - \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t^* \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t^* \end{bmatrix} \right\| \leq R_t := \frac{2\tilde{R}_t}{\sigma_d(\mathbf{M}_\lambda)}.$$

The third lemma states the convergence of inexact power iterations, paralleling [16, Theorem 4.1].

Lemma 9 (Convergence of inexact power iterations). Fix $\alpha > 0$. Consider the inexact power iterations described in Lemma 8.

- (crude regime) Let $t_1 = \lceil \frac{2}{\alpha} \log \left(\frac{4}{\mu' \alpha} \right) \rceil$. Fix $T \geq t_1$, and set $\tilde{\epsilon}(T) = \frac{\alpha^2 \cdot \sigma_d(\mathbf{M}_\lambda)}{64\kappa_\lambda} \left(\frac{2\kappa_\lambda - 1}{(2\kappa_\lambda)^T - 1} \right)^2$. Then we have
$$\frac{1}{2} \left[\mathbf{u}_T^\top \Sigma_{xx}^{\frac{1}{2}}, \mathbf{v}_T^\top \Sigma_{yy}^{\frac{1}{2}} \right] \mathbf{M}_\lambda \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_T \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_T \end{bmatrix} \geq (1 - \alpha) \cdot \sigma_1(\mathbf{M}_\lambda).$$
- (accurate regime) Let $t_2 = \lceil \frac{\delta(\mathbf{M}_\lambda)}{2} \log \left(\frac{2}{\mu' \alpha} \right) \rceil$. Fix $T \geq t_2$, and set $\tilde{\epsilon}(T) = \frac{\alpha^2 \cdot \sigma_d(\mathbf{M}_\lambda)}{64\kappa_\lambda} \left(\frac{2\kappa_\lambda - 1}{(2\kappa_\lambda)^T - 1} \right)^2$. Then we have
$$\frac{1}{4} (\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^* + \mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*)^2 \geq 1 - \alpha.$$

For brevity, let us define the following short-hands:

$$\begin{aligned} \tilde{\mathbf{r}}_t &= \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t \end{bmatrix}, & \mathbf{r}_t &= \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t \end{bmatrix}, & \bar{\mathbf{r}}_t &= \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \bar{\mathbf{u}}_t \\ \Sigma_{yy}^{\frac{1}{2}} \bar{\mathbf{v}}_t \end{bmatrix}, \\ \tilde{\mathbf{r}}_t^* &= \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t^* \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t^* \end{bmatrix}, & \mathbf{r}_t^* &= \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_t^* \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_t^* \end{bmatrix}, & \mathbf{r}^* &= \frac{1}{\sqrt{2}} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}^* \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}^* \end{bmatrix}. \end{aligned}$$

All these vectors are in \mathbb{R}^d and have length 1.

Observe that the matrix-vector multiplication (8) is equivalent to

$$\begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_t \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_t \end{bmatrix} \leftarrow \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} & \\ & \Sigma_{yy}^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix}^{-1} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} & \\ & \Sigma_{yy}^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}_{t-1} \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}_{t-1} \end{bmatrix},$$

and

$$\begin{aligned} & \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} & \\ & \Sigma_{yy}^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix}^{-1} \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} & \\ & \Sigma_{yy}^{\frac{1}{2}} \end{bmatrix} \\ &= \begin{bmatrix} \Sigma_{xx}^{-\frac{1}{2}} & \\ & \Sigma_{yy}^{-\frac{1}{2}} \end{bmatrix}^{-1} \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix}^{-1} \begin{bmatrix} \Sigma_{xx}^{-\frac{1}{2}} & \\ & \Sigma_{yy}^{-\frac{1}{2}} \end{bmatrix}^{-1} \\ &= \left(\begin{bmatrix} \Sigma_{xx}^{-\frac{1}{2}} & \\ & \Sigma_{yy}^{-\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \lambda \Sigma_{xx} & -\Sigma_{xy} \\ -\Sigma_{xy}^\top & \lambda \Sigma_{yy} \end{bmatrix} \begin{bmatrix} \Sigma_{xx}^{-\frac{1}{2}} & \\ & \Sigma_{yy}^{-\frac{1}{2}} \end{bmatrix} \right)^{-1} \\ &= \begin{bmatrix} \lambda \mathbf{I} & -\Sigma_{xx}^{-\frac{1}{2}} \Sigma_{xy} \Sigma_{yy}^{-\frac{1}{2}} \\ -\Sigma_{yy}^{-\frac{1}{2}} \Sigma_{xy}^\top \Sigma_{xx}^{-\frac{1}{2}} & \lambda \mathbf{I} \end{bmatrix}^{-1} \\ &= \mathbf{M}_\lambda. \end{aligned}$$

Then the updates for exact power iterations can be written as

$$\tilde{\mathbf{r}}_t^* \leftarrow \mathbf{M}_\lambda \mathbf{r}_{t-1}^*, \quad \mathbf{r}_t^* \leftarrow \tilde{\mathbf{r}}_t^* / \|\tilde{\mathbf{r}}_t^*\|, \quad t = 1, \dots,$$

and the updates for inexact power iterations can be written as

$$\tilde{\mathbf{r}}_t \approx \mathbf{M}_\lambda \mathbf{r}_{t-1}, \quad \mathbf{r}_t \leftarrow \tilde{\mathbf{r}}_t / \|\tilde{\mathbf{r}}_t\|, \quad t = 1, \dots$$

Note we have according to (18) that

$$\tilde{\epsilon} \geq (\tilde{\mathbf{r}}_t - \bar{\mathbf{r}}_t)^\top \mathbf{M}_\lambda^{-1} (\tilde{\mathbf{r}}_t - \bar{\mathbf{r}}_t) \geq \sigma_d(\mathbf{M}_\lambda^{-1}) \cdot \|\tilde{\mathbf{r}}_t - \bar{\mathbf{r}}_t\|^2 = \frac{1}{\sigma_1(\mathbf{M}_\lambda)} \cdot \|\tilde{\mathbf{r}}_t - \bar{\mathbf{r}}_t\|^2$$

or equivalently

$$\|\tilde{\mathbf{r}}_t - \bar{\mathbf{r}}_t\| \leq \sqrt{\sigma_1(\mathbf{M}_\lambda) \cdot \epsilon}. \quad (19)$$

Proof of Lemma 7. Recall that the eigenvectors of \mathbf{M}_λ are:

$$\lambda_1 := \frac{1}{\lambda - \rho_1} > \lambda_2 := \frac{1}{\lambda - \rho_2} \geq \dots \geq \lambda_{d-1} := \frac{1}{\lambda + \rho_2} \geq \lambda_d := \frac{1}{\lambda + \rho_1},$$

with corresponding eigenvectors

$$\mathbf{e}_1 = \mathbf{r}^* = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{a}_1 \\ \mathbf{b}_1 \end{bmatrix}, \mathbf{e}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{a}_2 \\ \mathbf{b}_2 \end{bmatrix}, \dots, \mathbf{e}_{d-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{a}_2 \\ -\mathbf{b}_2 \end{bmatrix}, \mathbf{e}_d = \frac{1}{\sqrt{2}} \begin{bmatrix} \mathbf{a}_1 \\ -\mathbf{b}_1 \end{bmatrix}.$$

By the update rule of exact power iterations, it holds that for $i = 1, \dots, d$ that

$$\begin{aligned} (\mathbf{e}_i^\top \mathbf{r}_t^*)^2 &= \frac{(\mathbf{e}_i^\top \mathbf{M}_\lambda^t \mathbf{r}_0^*)^2}{\|\mathbf{M}_\lambda^t \mathbf{r}_0^*\|^2} = \frac{(\mathbf{e}_i^\top \mathbf{M}_\lambda^t \mathbf{r}_0^*)^2}{(\mathbf{r}_0^*)^\top \mathbf{M}_\lambda^{2t} \mathbf{r}_0^*} = \frac{(\lambda_i^t \mathbf{e}_i^\top \mathbf{r}_0^*)^2}{\sum_{j=1}^d \lambda_j^{2t} (\mathbf{e}_j^\top \mathbf{r}_0^*)^2} = \frac{(\mathbf{e}_i^\top \mathbf{r}_0^*)^2}{\sum_{j=1}^d \left(\frac{\lambda_j}{\lambda_i}\right)^{2t} (\mathbf{e}_j^\top \mathbf{r}_0^*)^2} \\ &\leq \frac{(\mathbf{e}_i^\top \mathbf{r}_0^*)^2}{\left(\frac{\lambda_1}{\lambda_i}\right)^{2t} (\mathbf{e}_1^\top \mathbf{r}_0^*)^2} = \frac{(\mathbf{e}_i^\top \mathbf{r}_0^*)^2}{(\mathbf{e}_1^\top \mathbf{r}_0^*)^2} \left(\frac{\lambda_i}{\lambda_1}\right)^{2t} = \frac{(\mathbf{e}_i^\top \mathbf{r}_0^*)^2}{\tilde{\mu}} \left(1 - \frac{\lambda_1 - \lambda_i}{\lambda_1}\right)^{2t} \\ &\leq \frac{(\mathbf{e}_i^\top \mathbf{r}_0^*)^2}{\tilde{\mu}} \cdot \exp\left(-2 \frac{\lambda_1 - \lambda_i}{\lambda_1} t\right). \end{aligned}$$

Given $\delta \in (0, 1)$, define $S(\delta) = \{i : \lambda_i > (1 - \delta)\lambda_1\}$. For $\delta_1, \delta_2 \in (0, 1)$, define

$$T(\delta_1, \delta_2) := \lceil \frac{1}{2\delta_1} \log\left(\frac{1}{\tilde{\mu}\delta_2}\right) \rceil.$$

For all $i \notin S(\delta_1)$, when $t > T(\delta_1, \delta_2)$, it holds that $(\mathbf{e}_i^\top \mathbf{r}_t^*)^2 \leq \delta_2 (\mathbf{e}_i^\top \mathbf{r}_0^*)^2$, and thus in particular $\sum_{i \in S(\alpha/2)} (\mathbf{e}_i^\top \mathbf{r}_t^*)^2 \geq 1 - \delta_2$.

Part one (crude regime) of the lemma now follows by noticing that, by setting $\delta_1 = \delta_2 = \frac{\alpha}{2}$ we have that for $t \geq T\left(\frac{\alpha}{2}, \frac{\alpha}{2}\right)$, it holds that

$$(\mathbf{r}_t^*)^\top \mathbf{M}_\lambda \mathbf{r}_t^* = \sum_{i=1}^d \lambda_i (\mathbf{e}_i^\top \mathbf{r}_t^*)^2 \geq \sum_{i \in S(\alpha/2)} \left(1 - \frac{\alpha}{2}\right) \lambda_i (\mathbf{e}_i^\top \mathbf{r}_t^*)^2 \geq \left(1 - \frac{\alpha}{2}\right)^2 \lambda_1 \geq (1 - \alpha) \lambda_1.$$

For the second part (accurate regime) of the lemma, note that $S\left(\frac{\lambda_1 - \lambda_2}{\lambda_1}\right) = \{1\}$. Thus for all $t \geq T\left(\frac{\lambda_1 - \lambda_2}{\lambda_1}, \alpha\right)$, it holds that $(\mathbf{e}_1^\top \mathbf{r}_t^*)^2 \geq 1 - \alpha$.

□

Proof of Lemma 8. We prove the bound for unnormalized iterates by induction. The case for $t = 1$ holds trivially. For $t \geq 2$, we can bound the error of the unnormalized iterates using the exact solution to \tilde{h}_t :

$$\|\tilde{\mathbf{r}}_t - \tilde{\mathbf{r}}_t^*\| \leq \|\tilde{\mathbf{r}}_t - \bar{\mathbf{r}}_t\| + \|\bar{\mathbf{r}}_t - \tilde{\mathbf{r}}_t^*\|. \quad (20)$$

The second term of (20) is concerned with the error due to inexact target in the least squares problem

$h_t(\mathbf{u}, \mathbf{v})$ as $\begin{bmatrix} \mathbf{u}_{t-1} \\ \mathbf{v}_{t-1} \end{bmatrix}$ is different from $\begin{bmatrix} \mathbf{u}_{t-1}^* \\ \mathbf{v}_{t-1}^* \end{bmatrix}$. We can bound this term as

$$\begin{aligned} \|\bar{\mathbf{r}}_t - \tilde{\mathbf{r}}_t^*\| &= \|\mathbf{M}_\lambda \mathbf{r}_{t-1} - \mathbf{M}_\lambda \mathbf{r}_{t-1}^*\| \leq \|\mathbf{M}_\lambda\| \cdot \|\mathbf{r}_{t-1} - \mathbf{r}_{t-1}^*\| \\ &= \sigma_1(\mathbf{M}_\lambda) \cdot \|\mathbf{r}_{t-1} - \mathbf{r}_{t-1}^*\|. \end{aligned} \quad (21)$$

In view of the update rule of our algorithm and the triangle inequality, we have

$$\begin{aligned} &\|\mathbf{r}_{t-1} - \mathbf{r}_{t-1}^*\| \\ &\leq \left\| \frac{\tilde{\mathbf{r}}_{t-1}}{\|\tilde{\mathbf{r}}_{t-1}\|} - \frac{\tilde{\mathbf{r}}_{t-1}}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \right\| + \left\| \frac{\tilde{\mathbf{r}}_{t-1}}{\|\tilde{\mathbf{r}}_{t-1}^*\|} - \frac{\tilde{\mathbf{r}}_{t-1}^*}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \right\| \\ &= \|\tilde{\mathbf{r}}_{t-1}\| \left| \frac{1}{\|\tilde{\mathbf{r}}_{t-1}\|} - \frac{1}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \right| + \frac{1}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \|\tilde{\mathbf{r}}_{t-1} - \tilde{\mathbf{r}}_{t-1}^*\| \\ &= \frac{1}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \left| \|\tilde{\mathbf{r}}_{t-1}^*\| - \|\tilde{\mathbf{r}}_{t-1}\| \right| + \frac{1}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \|\tilde{\mathbf{r}}_{t-1} - \tilde{\mathbf{r}}_{t-1}^*\| \\ &\leq \frac{2}{\|\tilde{\mathbf{r}}_{t-1}^*\|} \|\tilde{\mathbf{r}}_{t-1} - \tilde{\mathbf{r}}_{t-1}^*\| \leq \frac{2\tilde{R}_{t-1}}{\|\tilde{\mathbf{r}}_{t-1}^*\|}. \end{aligned} \quad (22)$$

For $t \geq 2$, we have $\tilde{\mathbf{r}}_{t-1}^* = \mathbf{M}_\lambda \mathbf{r}_{t-2}^*$ and $\|\mathbf{r}_{t-2}^*\| = 1$, and thus

$$\|\tilde{\mathbf{r}}_{t-1}^*\| \geq \sigma_d(\mathbf{M}_\lambda).$$

Combining (20), (21) and (22) gives

$$\|\tilde{\mathbf{r}}_t - \tilde{\mathbf{r}}_t^*\| \leq \sqrt{\sigma_1(\mathbf{M}_\lambda) \cdot \epsilon} + 2\kappa_\lambda \tilde{R}_{t-1} = \tilde{R}_t.$$

The bound for normalized iterates follows from (22). \square

Proof of Lemma 9. For the first item (crude regime), observe that

$$\mathbf{r}_t^\top \mathbf{M}_\lambda \mathbf{r}_t = (\mathbf{r}_t^*)^\top \mathbf{M}_\lambda \mathbf{r}_t^* + ((\mathbf{r}_t^*)^\top \mathbf{M}_\lambda \mathbf{r}_t^* - \mathbf{r}_t^\top \mathbf{M}_\lambda \mathbf{r}_t), \quad (23)$$

and that

$$\begin{aligned} |(\mathbf{r}_t^*)^\top \mathbf{M}_\lambda (\mathbf{r}_t^*) - \mathbf{r}_t^\top \mathbf{M}_\lambda \mathbf{r}_t| &= \left| \left(\mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t^* + \mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t \right)^\top \left(\mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t^* - \mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t \right) \right| \\ &\leq \left\| \mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t^* + \mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t \right\| \left\| \mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t^* - \mathbf{M}_\lambda^{\frac{1}{2}} \mathbf{r}_t \right\| \\ &\leq \left\| \mathbf{M}_\lambda^{\frac{1}{2}} \right\| \|\mathbf{r}_t^* + \mathbf{r}_t\| \left\| \mathbf{M}_\lambda^{\frac{1}{2}} \right\| \|\mathbf{r}_t^* - \mathbf{r}_t\| \\ &\leq \|\mathbf{M}_\lambda\| (\|\mathbf{r}_t^*\| + \|\mathbf{r}_t\|) \|\mathbf{r}_t^* - \mathbf{r}_t\| \\ &= 2\sigma_1(\mathbf{M}_\lambda) \cdot \|\mathbf{r}_t^* - \mathbf{r}_t\|. \end{aligned}$$

Our choices of T and $\tilde{\epsilon}$ make sure that $(\mathbf{r}_T^*)^\top \mathbf{M}_\lambda \mathbf{r}_T^* \geq (1 - \frac{\alpha}{2}) \cdot \sigma_1(\mathbf{M}_\lambda)$ by Lemma 7 and that $\|\mathbf{r}_T^* - \mathbf{r}_T\| \leq R_T = \alpha/4$ by Lemma 8. Continuing from (23), we have

$$\mathbf{r}_T^\top \mathbf{M}_\lambda \mathbf{r}_T \geq \left(1 - \frac{\alpha}{2}\right) \cdot \sigma_1(\mathbf{M}_\lambda) - \frac{\alpha}{2} \cdot \sigma_1(\mathbf{M}_\lambda) = (1 - \alpha) \cdot \sigma_1(\mathbf{M}_\lambda).$$

For the second item (accurate regime), observe that

$$(\mathbf{r}_t^\top \mathbf{r}^*)^2 = ((\mathbf{r}_t^*)^\top \mathbf{r}^* + (\mathbf{r}_t - \mathbf{r}_t^*)^\top \mathbf{r}^*)^2 \geq ((\mathbf{r}_t^*)^\top \mathbf{r}^*)^2 - 2\|\mathbf{r}_t - \mathbf{r}_t^*\|. \quad (24)$$

Our choices of T and $\tilde{\epsilon}$ make sure that $((\mathbf{r}_T^*)^\top \mathbf{r}^*)^2 \geq 1 - \frac{\alpha}{2}$ by Lemma 7 and that $\|\mathbf{r}_T^* - \mathbf{r}_T\| \leq R_T = \alpha/4$ by Lemma 8. Continuing from (24), we have

$$(\mathbf{r}_T^\top \mathbf{r}^*)^2 \geq 1 - \frac{\alpha}{2} - \frac{\alpha}{2} = 1 - \alpha.$$

\square

F.2 Iteration complexity of Algorithm 3

Observe that, the **for** loops within the **repeat-until** loop, as well as the final **for** loop in Algorithm 3 are running inexact power iterations on $\mathbf{M}_{\lambda_{(s)}}$ and $\mathbf{M}_{\lambda_{(f)}}$ for m_1 and m_2 inexact matrix-vector multiplication respectively. And the convergence of inexact power iterations is provided by Lemma 8.

For each iteration of the **repeat-until** loop, we work in the crude regime and only require \mathbf{r}_{sm_1} to give a constant multiple estimate of $\mathbf{M}_{\lambda_{(s)}}$. The lemma below shows an important property of Δ_s which is used to locate $\lambda_{(f)}$, and the number of iterations needed to reach $\lambda_{(f)}$.

Lemma 10 (Iteration complexity of the **repeat-until** loop in Algorithm 3). Suppose that $\tilde{\Delta} \in [c_1\Delta, c_2\Delta]$ where $c_2 \leq 1$. Set $m_1 = \lceil 8 \log \left(\frac{16}{\mu'} \right) \rceil$ and $\tilde{\epsilon} \leq \frac{1}{3084} \left(\frac{\tilde{\Delta}}{18} \right)^{m_1-1}$ in Algorithm 3. Then for all $s \geq 1$ it holds that

$$\frac{1}{2}(\lambda_{(s-1)} - \rho_1) \leq \Delta_s \leq \lambda_{(s-1)} - \rho_1,$$

upon exiting this loop, the $\lambda_{(f)}$ satisfies

$$\rho_1 + \frac{\tilde{\Delta}}{4} \leq \lambda_{(f)} \leq \rho_1 + \frac{3\tilde{\Delta}}{2}, \quad (25)$$

and the number of iterations run by the **repeat-until** loop is $\log \left(\frac{1}{\Delta} \right)$.

Proof. Let $\bar{\sigma}$ be an upper bound of all $\sigma_1(\mathbf{M}_{\lambda_{(s)}})$ used in the **repeat-until** loop, i.e.,

$$\bar{\sigma} \geq \sigma_1(\mathbf{M}_{\lambda_{(s)}}), \quad s = 1, 2, \dots$$

And suppose for now that throughout the loop, $\tilde{\epsilon}$ satisfies

$$\sqrt{\bar{\sigma}\tilde{\epsilon}} \leq \frac{\sigma_1(\mathbf{M}_{\lambda_{(s-1)}})}{8}. \quad (26)$$

Set $\alpha = \frac{1}{4}$ in Lemma 8 (crude regime), and with our choice of m_1 and

$$\tilde{\epsilon} \leq \frac{\sigma_d(\mathbf{M}_{\lambda_{(s)}})}{1024\kappa_{\lambda_{(s)}}} \left(\frac{2\kappa_{\lambda_{(s)}} - 1}{(2\kappa_{\lambda_{(s)}})^{m_1} - 1} \right)^2, \quad (27)$$

we have

$$\mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} \geq \frac{3}{4} \sigma_1(\mathbf{M}_{\lambda_{(s-1)}}). \quad (28)$$

In view of the definition of the vector \mathbf{w}_s in Algorithm 3, and following the same argument in (18), we have

$$\left\| \frac{\mathbf{z}_s}{\sqrt{2}} - \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} \right\| \leq \sqrt{\sigma_1(\mathbf{M}_{\lambda_{(s-1)}}) \cdot \tilde{\epsilon}}$$

$$\text{where } \mathbf{z}_s = \begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} & \\ & \Sigma_{yy}^{\frac{1}{2}} \end{bmatrix} \mathbf{w}_s.$$

Then for every iteration of the **repeat-until** loop, it holds that

$$\begin{aligned} & \frac{1}{2} [\mathbf{u}_{sm_1}^\top \mathbf{v}_{sm_1}^\top] \begin{bmatrix} \Sigma_{xx} & \\ & \Sigma_{yy} \end{bmatrix} \mathbf{w}_s \\ &= \mathbf{r}_{sm_1}^\top \left(\frac{\mathbf{z}_s}{\sqrt{2}} \right) = \mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} + \mathbf{r}_{sm_1}^\top \left(\frac{\mathbf{z}_s}{\sqrt{2}} - \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} \right) \\ &\in \left[\mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} - \sqrt{\sigma_1(\mathbf{M}_{\lambda_{(s-1)}}) \cdot \tilde{\epsilon}}, \mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} + \sqrt{\sigma_1(\mathbf{M}_{\lambda_{(s-1)}}) \cdot \tilde{\epsilon}} \right] \\ &\in \left[\mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} - \sqrt{\bar{\sigma}\tilde{\epsilon}}, \mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} + \sqrt{\bar{\sigma}\tilde{\epsilon}} \right], \end{aligned}$$

where we have used the Cauchy-Schwarz inequality in the second step.

In view of (26) and (28), it follows that

$$\begin{aligned} & \frac{1}{2} [\mathbf{u}_{sm_1}^\top \mathbf{v}_{sm_1}^\top] \begin{bmatrix} \Sigma_{xx} & \\ & \Sigma_{yy} \end{bmatrix} \mathbf{w}_s - \sqrt{\sigma} \tilde{\epsilon} \\ & \in \left[\mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} - 2\sqrt{\sigma} \tilde{\epsilon}, \mathbf{r}_{sm_1}^\top \mathbf{M}_{\lambda_{(s-1)}} \mathbf{r}_{sm_1} \right] \\ & \in \left[\frac{1}{2} \sigma_1(\mathbf{M}_{\lambda_{(s-1)}}), \sigma_1(\mathbf{M}_{\lambda_{(s-1)}}) \right]. \end{aligned}$$

By the definition of Δ_s in Algorithm 3 and the fact that $\sigma_1(\mathbf{M}_{\lambda_{(s-1)}}) = \frac{1}{\lambda_{(s-1)} - \rho_1}$, we have

$$\Delta_s = \frac{1}{2} \cdot \frac{1}{\frac{1}{2} [\mathbf{u}_{sm_1}^\top \mathbf{v}_{sm_1}^\top] \begin{bmatrix} \Sigma_{xx} & \\ & \Sigma_{yy} \end{bmatrix} \mathbf{w}_s - \sqrt{\sigma} \tilde{\epsilon}} \in \left[\frac{1}{2} (\lambda_{(s-1)} - \rho_1), \lambda_{(s-1)} - \rho_1 \right]. \quad (29)$$

And as a result,

$$\lambda_{(s)} = \lambda_{(s-1)} - \frac{\Delta_s}{2} \geq \lambda_{(s-1)} - \frac{1}{2} (\lambda_{(s-1)} - \rho_1) = \frac{\lambda_{(s-1)} + \rho_1}{2},$$

and thus by induction (note $\lambda_{(0)} \geq \rho_1$) we have $\lambda_{(s)} \geq \rho_1$ throughout the **repeat-until** loop.

From (29) we also obtain

$$\lambda_{(s)} - \rho_1 = \lambda_{(s-1)} - \rho_1 - \frac{\Delta_s}{2} \leq \lambda_{(s-1)} - \rho_1 - \frac{1}{4} (\lambda_{(s-1)} - \rho_1) = \frac{3}{4} (\lambda_{(s-1)} - \rho_1).$$

To sum up, $\lambda_{(s)}$ approaches ρ_1 from above and the gap between $\lambda_{(s)}$ and ρ_1 reduces at the geometric rate of $\frac{3}{4}$. Thus after at most $t_3 = \lceil \log_{3/4} \left(\frac{\tilde{\Delta}}{\lambda_{(0)} - \rho_1} \right) \rceil \sim \mathcal{O} \left(\log \left(\frac{1}{\tilde{\Delta}} \right) \right)$ iterations, we reach a $\lambda_{(t_3)}$ such that $\lambda_{(t_3)} - \rho_1 \leq \tilde{\delta}$. And in view of (29), the **repeat-until** loop exits in the next iteration. Hence, the overall number of iterations is at most $t_3 + 1 = \mathcal{O} \left(\frac{1}{\tilde{\Delta}} \right)$.

We now analyze $\lambda_{(f)}$ and derive the interval it lies in. Note that $\Delta_f \leq \tilde{\Delta}$ and $\Delta_{f-1} > \tilde{\Delta}$ by the exiting condition. In view of (29), we have

$$\lambda_{(f)} - \rho_1 = \lambda_{(f-1)} - \rho_1 - \frac{\Delta_f}{2} \leq 2\Delta_f - \frac{\Delta_f}{2} = \frac{3\Delta_f}{2} \leq \frac{3\tilde{\Delta}}{2}.$$

On the other hand,

$$\lambda_{(f)} - \rho_1 = \lambda_{(f-1)} - \rho_1 - \frac{\Delta_f}{2} \geq \lambda_{(f-1)} - \rho_1 - \frac{1}{2} (\lambda_{(f-1)} - \rho_1) = \frac{1}{2} (\lambda_{(f-1)} - \rho_1). \quad (30)$$

If $f = 1$, then by our choice of $\lambda_{(0)}$ we have that $\lambda_{(f)} - \rho_1 \geq \tilde{\Delta}$. Otherwise, by unfolding (30) one more time, we have that

$$\lambda_{(f)} - \rho_1 \geq \frac{1}{4} (\lambda_{(f-2)} - \rho_1) \geq \frac{\Delta_{f-1}}{4} \geq \frac{\tilde{\Delta}}{4}.$$

Thus in both case, we have that $\lambda_{(f)} - \rho_1 \geq \frac{\tilde{\Delta}}{4}$ holds.

It remains to give an explicit bound on $\tilde{\epsilon}$ based on the two requirements (26) and (27). Since the $\lambda_{(s)}$ values are monotonically non-increasing and lower-bounded by $\rho_1 + \frac{\tilde{\Delta}}{4}$, we have

$$\max_s \sigma_1(\mathbf{M}_{\lambda_{(s)}}) = \sigma_1(\mathbf{M}_{\lambda_{(f)}}) = \frac{1}{\lambda_{(f)} - \rho_1} \leq \frac{4}{\tilde{\Delta}} =: \bar{\sigma},$$

and

$$\begin{aligned} \min_s \sigma_1(\mathbf{M}_{\lambda_{(s)}}) &= \sigma_1(\mathbf{M}_{\lambda_{(0)}}) = \frac{1}{\lambda_{(0)} - \rho_1} = \frac{1}{1 + \tilde{\Delta} - \rho_1} \\ &\geq \frac{1}{1 + c_2 \tilde{\Delta} - \tilde{\Delta}} \geq 1 + (1 - c_2) \tilde{\Delta} \geq 1 + \frac{1 - c_2}{c_2} \tilde{\Delta} := \underline{\sigma}, \end{aligned}$$

where the first inequality holds since by definition of Δ it follows that $\rho_1 = \rho_2 + \Delta \geq \Delta$.

Therefore, for the assumption (26) to hold, we just need

$$\left(\frac{\sigma}{8\sqrt{\bar{\sigma}}}\right)^2 = \frac{\left(1 + \frac{1-c_2}{c_2}\tilde{\Delta}\right)^2}{64 \cdot \frac{4}{\tilde{\Delta}}} \geq \frac{1}{64 \cdot \frac{4}{\tilde{\Delta}}} = \frac{\tilde{\Delta}}{256} \geq \tilde{\epsilon}. \quad (31)$$

We now derive a lower bound of the right hand side of (27). Notice

$$\kappa_{\lambda(s)} = \frac{\lambda(s) + \rho_1}{\lambda(s) - \rho_1} = 1 + \frac{2\rho_1}{\lambda(s) - \rho_1} \leq 1 + 2\rho_1\bar{\sigma} \leq 1 + 2\bar{\sigma} \leq \frac{9}{\tilde{\Delta}}. \quad (32)$$

On the other hand,

$$\sigma_d(\mathbf{M}_{\lambda(s)}) \geq \sigma_d(\mathbf{M}_{\lambda(0)}) = \frac{1}{\lambda(0) + \rho_1} = \frac{1}{1 + \tilde{\Delta} + \rho_1} \geq \frac{1}{3}.$$

As a result, we have

$$\begin{aligned} \frac{\sigma_d(\mathbf{M}_{\lambda(s)})}{1024\kappa_{\lambda(s)}} \left(\frac{2\kappa_{\lambda(s)} - 1}{(2\kappa_{\lambda(s)})^{m_1} - 1}\right)^2 &\geq \frac{1}{3084 \cdot \frac{9}{\tilde{\Delta}}} \left(\frac{2\frac{9}{\tilde{\Delta}} - 1}{\left(2\frac{9}{\tilde{\Delta}}\right)^{m_1} - 1}\right)^2 \geq \frac{\left(\frac{17}{\tilde{\Delta}}\right)^2}{3084 \cdot \frac{9}{\tilde{\Delta}} \cdot \left(\frac{18}{\tilde{\Delta}}\right)^{m_1}} \\ &\geq \frac{1}{3084} \left(\frac{\tilde{\Delta}}{18}\right)^{m_1-1}. \end{aligned} \quad (33)$$

Our final bound on $\tilde{\epsilon}$ chooses the smaller of (31) and (33). \square

For the final **for** loop of Algorithm 3, we work in the accurate regime of power iterations.

Lemma 11 (Iteration complexity of the final **for** loop in Algorithm 3). Suppose that $\tilde{\Delta} \in [c_1\Delta, c_2\Delta]$ where $c_2 \leq 1$. Set $m_2 = \lceil \frac{5}{4} \log \left(\frac{128}{\mu\eta^2} \right) \rceil$ and $\tilde{\epsilon} \leq \frac{\eta^4}{4^{10}} \left(\frac{\tilde{\Delta}}{18} \right)^{m_2-1}$ in Algorithm 3. Then the $(\mathbf{u}_T, \mathbf{v}_T)$ output by Phase I satisfies

$$\frac{1}{4}(\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^* + \mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*)^2 \geq 1 - \frac{\eta^2}{64}. \quad (34)$$

Proof. Notice when $\lambda = \rho_1 + c(\rho_1 - \rho_2)$, we have

$$\delta(\mathbf{M}_\lambda) = \frac{\sigma_1(\mathbf{M}_\lambda)}{\sigma_1(\mathbf{M}_\lambda) - \sigma_2(\mathbf{M}_\lambda)} = \frac{\frac{1}{\lambda - \rho_1}}{\frac{1}{\lambda - \rho_1} - \frac{1}{\lambda - \rho_2}} = \frac{\lambda - \rho_2}{\rho_1 - \rho_2} = \frac{\rho_1 + c(\rho_1 - \rho_2) - \rho_2}{\rho_1 - \rho_2} = c + 1.$$

In view of (25), $\lambda_{(f)} - \rho_1 \leq \frac{3}{2}\tilde{\Delta} \leq \frac{3c_2}{2}\Delta \leq \frac{3}{2}\Delta$, and thus $\delta(\mathbf{M}_{\lambda_{(f)}}) \leq \frac{5}{2}$.

Set $\alpha = \frac{\eta^2}{64}$ in Lemma 8 (accurate regime), and with our choice of m_2 and

$$\tilde{\epsilon} \leq \frac{\eta^4 \cdot \sigma_d(\mathbf{M}_{\lambda_{(f)}})}{64^3 \cdot \kappa_{\lambda_{(f)}}} \left(\frac{2\kappa_{\lambda_{(f)}} - 1}{(2\kappa_{\lambda_{(f)}})^{m_2} - 1}\right)^2, \quad (35)$$

we are guaranteed to obtain the desired alignment.

We now give a lower bound of the right hand side of (35). First,

$$\sigma_d(\mathbf{M}_{\lambda_{(f)}}) = \frac{1}{\lambda_{(f)} + \rho_1} \geq \frac{1}{\rho_1 + \frac{3}{2}\Delta + \rho_1} \geq \frac{1}{4}.$$

Recall that we have proved in (32) that $\kappa_{\lambda_{(f)}} \leq \frac{9}{\tilde{\Delta}}$. Following a derivation similar to that of (33), we have

$$\frac{\eta^4 \cdot \sigma_d(\mathbf{M}_{\lambda_{(f)}})}{64^3 \cdot \kappa_{\lambda_{(f)}}} \left(\frac{2\kappa_{\lambda_{(f)}} - 1}{(2\kappa_{\lambda_{(f)}})^{m_2} - 1}\right)^2 \geq \frac{\eta^4}{4^{10}} \left(\frac{\tilde{\Delta}}{18}\right)^{m_2-1}, \quad (36)$$

and this explains the ϵ we set in the lemma. \square

Proof of Theorem 4. As shown in Lemma 11, the **repeat-until** loop runs $\mathcal{O}\left(\log\left(\frac{1}{\Delta}\right)\right) \sim \mathcal{O}\left(\log\left(\frac{1}{\Delta}\right)\right)$ iterations, and inside each iteration, we run m_1 approximate matrix-vector multiplications. On the other hand, the final **for** loop runs m_2 approximate matrix-vector multiplications. By the definitions of m_1 and m_2 , the total number of invocations of approximate matrix-vector multiplications/least squares problems is

$$m_1 \cdot \log\left(\frac{1}{\Delta}\right) + m_2 \sim \mathcal{O}\left(\log\left(\frac{1}{\mu}\right) \log\left(\frac{1}{\Delta}\right) + \log\left(\frac{1}{\mu\eta^2}\right)\right) \sim \tilde{\mathcal{O}}(1).$$

□

G Proof of Theorem 5

Proof. Notice that the eigenvectors of \mathbf{M}_λ form an orthonormal bases of $\mathbb{R}^{d_x+d_y}$. Thus when (34) holds, i.e., the alignment between $\begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_T \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_T \end{bmatrix}$ and $\begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}^* \\ \Sigma_{yy}^{\frac{1}{2}} \mathbf{v}^* \end{bmatrix}$ is large, the alignments between

$\begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_T \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_T \end{bmatrix}$ and other eigenvectors have to be small. In particular, the alignment between $\begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \tilde{\mathbf{u}}_T \\ \Sigma_{yy}^{\frac{1}{2}} \tilde{\mathbf{v}}_T \end{bmatrix}$ and the tailing eigenvector $\begin{bmatrix} \Sigma_{xx}^{\frac{1}{2}} \mathbf{u}^* \\ -\Sigma_{yy}^{\frac{1}{2}} \mathbf{v}^* \end{bmatrix}$ has to be small:

$$(\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^* - \mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*)^2 \leq \frac{\eta^2}{16}. \quad (37)$$

From (37) and (34), we have respectively

$$-\frac{\eta}{4} \leq |\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^*| - |\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*| \leq \frac{\eta}{4},$$

$$|\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^*| + |\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*| \geq 2\sqrt{1 - \frac{\eta^2}{64}} \geq 2\left(1 - \frac{\eta}{8}\right)$$

where we have used the fact that $\sqrt{1-x} \geq 1 - \sqrt{x}$ for $x \in [0, 1]$ in the second inequality.

Averaging the above two inequalities gives

$$|\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^*| \geq 1 - \frac{\eta}{4}, \quad |\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*| \geq 1 - \frac{\eta}{4}.$$

Finally,

$$\begin{aligned} (\hat{\mathbf{u}}^\top \Sigma_{xx} \mathbf{u}^*)^2 + (\hat{\mathbf{v}}^\top \Sigma_{yy} \mathbf{v}^*)^2 &= \frac{(\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}^*)^2}{\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}_T} + \frac{(\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}^*)^2}{\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}_T} \\ &\geq \left(1 - \frac{\eta}{4}\right)^2 \left(\frac{1}{\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}_T} + \frac{1}{\mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}_T}\right) \\ &\geq \left(1 - \frac{\eta}{4}\right)^2 \frac{4}{\mathbf{u}_T^\top \Sigma_{xx} \mathbf{u}_T + \mathbf{v}_T^\top \Sigma_{yy} \mathbf{v}_T} \\ &\geq 2\left(1 - \frac{\eta}{2}\right) = 2 - \eta \end{aligned}$$

where we have used the fact that $\frac{1}{x} + \frac{1}{y} \geq \frac{4}{x+y}$ in the first inequality, and (10) in the second inequality. Then the theorem follows from the fact that $(\hat{\mathbf{u}}^\top \Sigma_{xx} \mathbf{u}^*)^2$ and $(\hat{\mathbf{v}}^\top \Sigma_{yy} \mathbf{v}^*)^2$ can be at most 1. □

H Condition number of h_t for SVRG

Lemma 12. Throughout Algorithm 3, the condition number of h_t for SVRG is at most $\frac{9/c}{\Delta} \tilde{\kappa}$, where

$$\tilde{\kappa} := \frac{\max_i \max \left(\|\mathbf{x}_i\|^2, \|\mathbf{y}_i\|^2 \right)}{\min(\sigma_{\min}(\Sigma_{xx}), \sigma_{\min}(\Sigma_{yy}))}.$$

Proof. The gradient Lipschitz constant of $h_t^i(\mathbf{u}, \mathbf{v})$ is bounded by the largest eigenvalue (in absolute value) of its Hessian⁸

$$\mathbf{Q}_\lambda^i = \begin{bmatrix} \lambda \mathbf{x}_i \mathbf{x}_i^\top & -\mathbf{x}_i \mathbf{y}_i^\top \\ -\mathbf{y}_i \mathbf{x}_i^\top & \lambda \mathbf{y}_i \mathbf{y}_i^\top \end{bmatrix},$$

and the largest eigenvalue is defined as

$$\max_{\mathbf{g}_x \in \mathbb{R}^{d_x}, \mathbf{g}_y \in \mathbb{R}^{d_y}} \beta := \left| [\mathbf{g}_x^\top, \mathbf{g}_y^\top] \mathbf{Q}_\lambda^i \begin{bmatrix} \mathbf{g}_x \\ \mathbf{g}_y \end{bmatrix} \right| \quad \text{s.t.} \quad \|\mathbf{g}_x\|^2 + \|\mathbf{g}_y\|^2 = 1.$$

We have

$$\begin{aligned} \beta &= |\lambda(\mathbf{g}_x^\top \mathbf{x}_i)^2 + \lambda(\mathbf{g}_y^\top \mathbf{y}_i)^2 - 2(\mathbf{g}_x^\top \mathbf{x}_i)(\mathbf{g}_y^\top \mathbf{y}_i)| \\ &\leq \lambda(\mathbf{g}_x^\top \mathbf{x}_i)^2 + \lambda(\mathbf{g}_y^\top \mathbf{y}_i)^2 + 2|\mathbf{g}_x^\top \mathbf{x}_i| |\mathbf{g}_y^\top \mathbf{y}_i| \\ &\leq \lambda(\mathbf{g}_x^\top \mathbf{x}_i)^2 + \lambda(\mathbf{g}_y^\top \mathbf{y}_i)^2 + (\mathbf{g}_x^\top \mathbf{x}_i)^2 + (\mathbf{g}_y^\top \mathbf{y}_i)^2 \\ &= (\lambda + 1) ((\mathbf{g}_x^\top \mathbf{x}_i)^2 + (\mathbf{g}_y^\top \mathbf{y}_i)^2) \\ &\leq (\lambda + 1) (\|\mathbf{g}_x\|^2 \|\mathbf{x}_i\|^2 + \|\mathbf{g}_y\|^2 \|\mathbf{y}_i\|^2) \\ &\leq (\lambda + 1) \max(\|\mathbf{x}_i\|^2, \|\mathbf{y}_i\|^2) \end{aligned}$$

where we have used the Cauchy-Schwarz inequality and the constraint in the third and the last inequality respectively.

It only remains to bound $\frac{\lambda+1}{\lambda-\rho}$. Note that we have shown in Lemma 10 that $\lambda \geq \rho_1 + \frac{\tilde{\Delta}}{4}$ throughout Algorithm 3, and thus

$$\frac{\lambda+1}{\lambda-\rho} = 1 + \frac{1+\rho}{\lambda-\rho} \leq 1 + \frac{2}{\lambda-\rho} \leq 1 + 2\frac{4}{\tilde{\Delta}} \leq \frac{9}{\tilde{\Delta}} \leq \frac{9/c_1}{\Delta}.$$

□

I More details of the experiments

The statistics of these datasets are summarized in Table 2. These datasets have also been used by [3, 4] for demonstrating their stochastic CCA algorithms.

Table 2: Brief summary of datasets.

Datasets	Description	d_x	d_y	N
Mediamill	Image and its labels	100	120	30,000
JW11	Acoustic and articulation measurements	273	112	30,000
MNIST	Left and right halves of images	392	392	60,000

We now provide additional details for the experiments. For **s-AppGrad**, both gradient and normalization steps are estimated with mini-batches of 100 samples (the authors of [3] suggest that the mini-batch size shall be at least the same magnitude as the dimensionality of the CCA projection). For **SI-VR** and **SI-AVR**, within the **repeat-until** loop, we apply SVRG with $M = 2$ epochs to approximately find the top eigenvector \mathbf{w}_s , and SVRG with $M = 2$ epochs to approximately calculate its top eigenvalue of $\mathbf{M}_{\lambda(s)}$ as $\mathbf{w}_s^T \mathbf{M}_{\lambda(s)} \mathbf{w}_s$. We exit the **repeat-until** loop when $\Delta_s \leq 0.06$. Afterwards, for the fixed $\lambda_{(f)}$, we apply SVRG to solve every least squares problems with $M = 4$ epochs. Each epoch of SVRG includes a batch gradient evaluation and $m = N$ stochastic gradient steps. We set the step size according to the smoothness for each least squares solver, i.e., $\frac{1}{\sigma_{\max}(\Sigma_{xx})}$ for GD/AGD in AppGrad/s-AppGrad/CCALin, and $\frac{1}{\max_i \|\mathbf{x}_i\|^2}$ for SVRG/ASVRG in our algorithms.

⁸We omit the regularization terms, which are typically very small, to have concise expressions.

J Other related work

Recent years have witnessed continuous efforts to scale up fundamental methods such as principal component analysis (PCA) and partial least squares with stochastic/online updates [22, 23, 24, 25, 5, 16, 17]. But as pointed out by [23], the CCA objective is more challenging due to the constraints.

[26] proposed an adaptive CCA algorithm with efficient online updates based on matrix manifolds defined by the constraints. However, the goal of their algorithm is anomaly detection for streaming data with a varying distribution, rather than to optimize the CCA objective on a given dataset. Similar to our algorithms, the stochastic CCA algorithms of [3, 4] are motivated by the ALS formulation. [5] proposed a stochastic algorithm based on the Lagrangian formulation of the objective (1). None of these online/stochastic algorithms have rigorous global convergence guarantee.