Derivative of the first order SVD

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Consider computing the first order SVD expansion. By the Eckart–Young–Mirsky theorem, this is equivalent to solving

$$\underset{\sigma,\, u,\, v}{\text{minimize}}\ \tfrac{1}{2}\|A - \sigma u v^\top\|_F^2 \quad \text{s.t.} \quad \|u\| = 1 \quad \text{and} \quad \|v\| = 1$$

Any triplet $(\sigma,\, u,\, v)$ for a **unique** singular value satisfies

$$\begin{aligned} \sigma &= u^\top A v \\ A v &= \sigma u \\ A^\top u &= \sigma v \end{aligned}$$

from this we can derive

$$\begin{aligned} \Delta\sigma &= \Delta u^\top A v + u^\top \Delta A v + u^\top A \Delta v \\ &= \Delta u^\top u + u^\top \Delta A v + v^\top \Delta v \\ &= u^\top \Delta A v \end{aligned}$$

Where in the last step we used $\Delta u \perp u$ and $\Delta v \perp v$, which follows from the side condition. Further we have:

$$\begin{aligned} \Delta A v + A \Delta v &= \Delta\sigma u + \sigma \Delta u \\ \Delta A^\top u + A^\top \Delta u &= \Delta\sigma v + \sigma \Delta v \end{aligned} \iff \underbrace{\begin{bmatrix} \sigma \mathbb{I}_m & -A \\ -A^\top & \sigma \mathbb{I}_n \end{bmatrix}}_{=:K} \cdot \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix} = \begin{bmatrix} \Delta A v - \Delta\sigma u \\ \Delta A^\top u - \Delta\sigma v \end{bmatrix}$$

1 The VJP

The last equation allows us to compute the VJP at ease:

$$\begin{aligned} \left\langle \begin{bmatrix} \phi \\ \psi \end{bmatrix} \,\middle|\, \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix} \right\rangle &= \left\langle \begin{bmatrix} \phi \\ \psi \end{bmatrix} \,\middle|\, K^{-1} \begin{bmatrix} \Delta A v - \Delta\sigma u \\ \Delta A^\top u - \Delta\sigma v \end{bmatrix} \right\rangle \\ &= \left\langle K^{-\top} \begin{bmatrix} \phi \\ \psi \end{bmatrix} \,\middle|\, \begin{bmatrix} \Delta A v - \Delta\sigma u \\ \Delta A^\top u - \Delta\sigma v \end{bmatrix} \right\rangle \\ &= \left\langle \begin{bmatrix} \tilde\phi \\ \tilde\psi \end{bmatrix} \,\middle|\, \begin{bmatrix} \Delta A v - \Delta\sigma u \\ \Delta A^\top u - \Delta\sigma v \end{bmatrix} \right\rangle \end{aligned}$$

Now, we compute the terms individually:

$$\begin{aligned}\langle\tilde{\phi} \mid \Delta A v - \Delta\sigma u\rangle &= \langle\tilde{\phi} v^\top \mid \Delta A\rangle - \langle u^\top \tilde{\phi} \mid \Delta\sigma\rangle \\ &= \langle\tilde{\phi} v^\top \mid \Delta A\rangle - \langle u^\top \tilde{\phi} \mid u^\top \Delta A v\rangle \\ &= \langle(\mathbb{I}_m - uu^\top)\tilde{\phi} v^\top \mid \Delta A\rangle\end{aligned}$$

And for the second term we get

$$\begin{aligned}\langle\tilde{\psi} \mid \Delta A^\top u - \Delta\sigma v\rangle &= \langle\tilde{\psi} u^\top \mid \Delta A^\top\rangle - \langle v^\top \tilde{\psi} \mid \Delta\sigma\rangle \\ &= \langle u\tilde{\psi}^\top \mid \Delta A\rangle - \langle \tilde{\psi}^\top v \mid u^\top \Delta A v\rangle \\ &= \langle u\tilde{\psi}(\mathbb{I}_n - vv^\top) \mid \Delta A\rangle\end{aligned}$$

Using the formula for inverting a block-matrix, we can give an explicit solution to $K^{-\top}$:

$$\begin{aligned}\begin{bmatrix}\sigma\mathbb{I}_m & -A \\ -A^\top & \sigma\mathbb{I}_n\end{bmatrix}^{-1} &= \begin{bmatrix}(\sigma\mathbb{I}_m - \frac{1}{\sigma}AA^\top)^{-1} & \mathbf{0}_{m\times n} \\ \mathbf{0}_{n\times m} & (\sigma\mathbb{I}_n - \frac{1}{\sigma}A^\top A)^{-1}\end{bmatrix} \cdot \begin{bmatrix}\mathbb{I}_m & \frac{1}{\sigma}A \\ \frac{1}{\sigma}A^\top & \mathbb{I}_n\end{bmatrix} \\ &= \begin{bmatrix}\frac{1}{\sigma}(\mathbb{I}_m - \frac{1}{\sigma^2}AA^\top)^{-1} & \frac{1}{\sigma^2}(\mathbb{I}_m - \frac{1}{\sigma^2}AA^\top)^{-1}A \\ \frac{1}{\sigma^2}(\mathbb{I}_n - \frac{1}{\sigma^2}A^\top A)^{-1}A^\top & \frac{1}{\sigma}(\mathbb{I}_n - \frac{1}{\sigma^2}A^\top A)^{-1}\end{bmatrix} \\ &= \frac{1}{\sigma}\begin{bmatrix}(\mathbb{I}_m - \tilde{A}\tilde{A}^\top)^{-1} & (\mathbb{I}_m - \tilde{A}\tilde{A}^\top)^{-1}\tilde{A} \\ (\mathbb{I}_n - \tilde{A}^\top\tilde{A})^{-1}\tilde{A}^\top & (\mathbb{I}_n - \tilde{A}^\top\tilde{A})^{-1}\end{bmatrix}\end{aligned}$$

And we see it's basically projection operators with respect to the image/kernel of $\tilde{A} = \frac{1}{\sigma}A$. In summary, we obtain the following formula for the VJP:

$$\begin{aligned}\begin{bmatrix}\sigma\mathbb{I}_m & -A \\ -A^\top & \sigma\mathbb{I}_n\end{bmatrix}^{-\top}\begin{bmatrix}\tilde{\phi} \\ \tilde{\psi}\end{bmatrix} = \begin{bmatrix}\phi \\ \psi\end{bmatrix} &\iff \begin{bmatrix}\tilde{\phi} \\ \tilde{\psi}\end{bmatrix} = \frac{1}{\sigma}\begin{bmatrix}(\mathbb{I}_m - \tilde{A}\tilde{A}^\top)^{-1} & (\mathbb{I}_m - \tilde{A}\tilde{A}^\top)^{-1}\tilde{A} \\ (\mathbb{I}_n - \tilde{A}^\top\tilde{A})^{-1}\tilde{A}^\top & (\mathbb{I}_n - \tilde{A}^\top\tilde{A})^{-1}\end{bmatrix}^\top\begin{bmatrix}\phi \\ \psi\end{bmatrix} \\ &\iff \begin{bmatrix}\tilde{\phi} \\ \tilde{\psi}\end{bmatrix} = \frac{1}{\sigma}\begin{bmatrix}(\mathbb{I}_m - \tilde{A}\tilde{A}^\top)^{-1} & \tilde{A}(\mathbb{I}_n - \tilde{A}^\top\tilde{A})^{-1} \\ \tilde{A}^\top(\mathbb{I}_m - \tilde{A}\tilde{A}^\top)^{-1} & (\mathbb{I}_n - \tilde{A}^\top\tilde{A})^{-1}\end{bmatrix}\begin{bmatrix}\phi \\ \psi\end{bmatrix}\end{aligned}$$

Thus, we need to solve 4 linear systems:

$$\begin{aligned}(\mathbb{I}_m - \tilde{A}\tilde{A}^\top)x &= \phi & \qquad (\mathbb{I}_n - \tilde{A}^\top\tilde{A})y &= \tilde{A}\psi \\ (\mathbb{I}_m - \tilde{A}\tilde{A}^\top)z &= \tilde{A}^\top\phi & \qquad (\mathbb{I}_n - \tilde{A}^\top\tilde{A})w &= \psi\end{aligned}$$

Then $\tilde{\phi} = \frac{1}{\sigma}(x+y)$ and $\tilde{\psi} = \frac{1}{\sigma}(z+w)$, and the VJP are given by the previous equations:

$$\begin{aligned}\xi^\top\frac{\partial\sigma}{\partial A} &= \xi uv^\top \\ \phi^\top\frac{\partial u}{\partial A} &= (\mathbb{I}_m - uu^\top)\tilde{\phi}v^\top \\ \psi^\top\frac{\partial v}{\partial A} &= u\tilde{\psi}(\mathbb{I}_n - vv^\top)\end{aligned}$$