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

$$\underset{\sigma, u, v}{\text{minimize}} \, \tfrac{1}{2} \|A - \sigma u v^\top\|_F^2 \quad \text{s.t.} \quad \|u\| = 1 \quad \text{and} \quad \|v\| = 1 \quad \text{and} \quad \sigma \geq 0$$

Equivalently this may be formalized as

$$\sigma = \max_{u, v} u^{\top} A v$$
 s.t. $||u|| = 1$ and $||v|| = 1$

Which is a non-convex quadratically constrained quadratic program (QCQP)

$$\sigma = \max_{u,v} \frac{1}{2} \begin{bmatrix} u \\ v \end{bmatrix}^{\top} \cdot \begin{bmatrix} \mathbf{0}_{m \times m} & A \\ A^{\top} & \mathbf{0}_{n \times n} \end{bmatrix} \cdot \begin{bmatrix} u \\ v \end{bmatrix} \text{ s.t. } \begin{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}^{\top} \cdot \begin{bmatrix} \mathbb{I}_{m} & \mathbf{0}_{m \times n} \\ \mathbf{0}_{n \times m} & \mathbf{0}_{n \times n} \end{bmatrix} \cdot \begin{bmatrix} u \\ v \end{bmatrix} = 1$$
$$\begin{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}^{\top} \cdot \begin{bmatrix} \mathbf{0}_{m \times m} & \mathbf{0}_{m \times n} \\ \mathbf{0}_{n \times m} & \mathbb{I}_{n} \end{bmatrix} \cdot \begin{bmatrix} u \\ v \end{bmatrix} = 1$$

The Jacobian and Lagrangian The derivative of the objective function is

$$\mathbf{J}_f(A, \begin{bmatrix} \sigma \\ u \\ v \end{bmatrix}) = \begin{bmatrix} \sigma - u^\top A v & \sigma - u^\top A v \\ A - \sigma u v^\top & \sigma^2 u - \sigma A v \\ \sigma^2 v - \sigma A^\top u \end{bmatrix} \implies \mathbf{H}_f(\begin{bmatrix} \sigma \\ u \\ v \end{bmatrix}) = \begin{bmatrix} 1 & 2\sigma u - A v & 2\sigma v - A^\top u \\ -A v & \sigma^2 \mathbb{I}_m & -\sigma A \\ -A^\top u & -\sigma A^\top & \sigma^2 \mathbb{I}_n \end{bmatrix}$$

Consider the function

$$f(A, \begin{bmatrix} \sigma \\ u \\ v \end{bmatrix}) = \begin{pmatrix} \sigma - u^{\top} A v \\ \sigma^{2} u - \sigma A v \\ \sigma^{2} v - \sigma A^{\top} u \end{pmatrix} \equiv \mathbf{0} \implies \mathbf{J}_{f}(A, \begin{bmatrix} \sigma \\ u \\ v \end{bmatrix}) = \begin{bmatrix} -\xi v u^{\top} & 1 & 2\sigma u - A v & 2\sigma v - A^{\top} u \\ -\sigma v \phi^{\top} & -A v & \sigma^{2} \mathbb{I}_{m} & -\sigma A \\ -\sigma u \psi^{\top} & -A^{\top} u & -\sigma A^{\top} & \sigma^{2} \mathbb{I}_{n} \end{bmatrix}$$

Thus, gradient descent schema is

$$\sigma' = \sigma - \eta_{\sigma}(\sigma - u^{\top} A v)$$

$$u' = u - \eta_{u}(\sigma^{2} u - \sigma A v)$$

$$v' = v - \eta_{v}(\sigma^{2} v - \sigma A^{\top} u)$$

And the newton step with diagonal approximation of the hessian:

$$\sigma' = \sigma - 1(\sigma - u^{\top} A v) = u^{\top} A v$$

$$u' = u - \frac{1}{\sigma^2} (\sigma^2 u - \sigma A v) = \frac{1}{\sigma} A v$$

$$v' = v - \frac{1}{\sigma^2} (\sigma^2 v - \sigma A^{\top} u) = \frac{1}{\sigma} A^{\top} u$$

1 Analysis of the backward

At the equilibrium point, we have:

$$\sigma = u^{\top} A v$$
 $A v = \sigma u$ $A^{\top} u = \sigma v$ $u^{\top} u = 1$ $v^{\top} v = 1$

Note that this states that σ is an eigenvalue:

$$\begin{bmatrix} 0 & A \\ A^{\top} & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \sigma \begin{bmatrix} u \\ v \end{bmatrix}$$

In particular, Rayleigh iteration could be useful. from this we can derive

$$\Delta \sigma = \Delta u^{\top} A v + u^{\top} \Delta A v + u^{\top} A \Delta v = \Delta u^{\top} u + u^{\top} \Delta A v + v^{\top} \Delta v = u^{\top} \Delta A v$$

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:

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

which allows us to express Δu and Δv in terms of ΔA . The constraints yield

$$u^{\top} \Delta u + \Delta u^{\top} u = 0 \iff u \perp \Delta u$$
$$v^{\top} \Delta v + \Delta v^{\top} v = 0 \iff v \perp \Delta v$$

We can augment the original system with these:

$$\underbrace{\begin{bmatrix} \sigma \mathbb{I}_m & -A \\ -A^\top & \sigma \mathbb{I}_n \\ u^\top & \mathbf{0}_n^\top \\ \mathbf{0}_m^\top & v^\top \end{bmatrix}}_{=:\widetilde{K}} \cdot \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix} = \underbrace{\begin{bmatrix} \Delta Av - \Delta \sigma u \\ \Delta A^\top u - \Delta \sigma v \\ 0 \\ 0 \end{bmatrix}}_{=:\widetilde{c}}$$

2 VJP with modified K matrix

$$\begin{split} \left\langle \begin{bmatrix} \phi \\ \psi \end{bmatrix} \mid \begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix} \right\rangle &= \left\langle \begin{bmatrix} \phi \\ \psi \end{bmatrix} \mid \widetilde{K}^{-1} \widetilde{c} \right\rangle \\ &= \left\langle \widetilde{K}^{-\top} \begin{bmatrix} \phi \\ \psi \end{bmatrix} \mid \widetilde{c} \right\rangle \\ &= \left\langle \begin{bmatrix} \sigma \mathbb{I}_m & -A & u & \mathbf{0}_m \\ -A^\top & \sigma \mathbb{I}_n & \mathbf{0}_n & v \end{bmatrix}^{-1} \begin{bmatrix} \phi \\ \psi \end{bmatrix} \mid \begin{bmatrix} \overset{\Delta A v - \Delta \sigma u}{\Delta A^\top u - \Delta \sigma v} \end{bmatrix} \right\rangle \\ &= \left\langle \begin{bmatrix} \sigma \mathbb{I}_m & -A & u & \mathbf{0}_m \\ -A^\top & \sigma \mathbb{I}_n & \mathbf{0}_n & v \end{bmatrix} \begin{bmatrix} \overset{p}{q} \\ \overset{\lambda}{\mu} \end{bmatrix} = \begin{bmatrix} \phi \\ \psi \end{bmatrix} \mid \begin{bmatrix} \overset{\Delta A v - \Delta \sigma u}{\Delta A^\top u - \Delta \sigma v} \end{bmatrix} \right\rangle \end{split}$$

2.1 Augmented block inversion

NOTE: Tested this and the issue is that it vastly increases the condition number!

We use the technique Column-wise partitioning in over-determined least squares.

$$\begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = d \iff x = \begin{bmatrix} A & B \end{bmatrix}^{\dagger} d = \begin{bmatrix} (P_B^{\perp} A)^{\dagger} \\ (P_A^{\perp} B)^{\dagger} \end{bmatrix} d$$

In particular, in our case this means that the relevant part of the solution is

$$\begin{bmatrix} p \\ q \end{bmatrix} = (P_B^{\perp} K)^{\star} \begin{bmatrix} \phi \\ \psi \end{bmatrix}$$

Here

$$\begin{split} P_B^\perp &= \mathbb{I} - BB^+ \\ &= \mathbb{I} - B(B^TB)^{-1}B^\top \\ &= \mathbb{I} - \begin{bmatrix} u & 0 \\ 0 & v \end{bmatrix} \begin{pmatrix} \begin{bmatrix} u^\top & 0^\top \\ 0^\top & v^\top \end{bmatrix} \begin{bmatrix} u & 0 \\ 0 & v \end{bmatrix} \end{pmatrix}^{-1} \begin{bmatrix} u^\top & 0^\top \\ 0^\top & v^\top \end{bmatrix} \\ &= \mathbb{I} - \begin{bmatrix} u & 0 \\ 0 & v \end{bmatrix} \begin{pmatrix} \begin{bmatrix} u^\top & 0^\top \\ 0^\top & v^\top \end{bmatrix} \begin{bmatrix} u & 0 \\ 0 & v \end{bmatrix} \end{pmatrix}^{-1} \begin{bmatrix} u^\top & 0^\top \\ 0^\top & v^\top \end{bmatrix} \\ &= \mathbb{I} - \begin{bmatrix} u & 0 \\ 0 & v \end{bmatrix} \begin{bmatrix} 1/\|u\|^2 & 0 \\ 0 & 1/\|v\|^2 \end{bmatrix} \begin{bmatrix} u^\top & 0^\top \\ 0^\top & v^\top \end{bmatrix} \\ &= \mathbb{I} - \begin{bmatrix} u & 0 \\ 0 & v \end{bmatrix} \begin{bmatrix} 1/\|u\|^2 & 0 \\ 0 & 1/\|v\|^2 \end{bmatrix} \begin{bmatrix} u^\top & 0^\top \\ 0^\top & v^\top \end{bmatrix} \\ &= \begin{bmatrix} \mathbb{I}_m - uu^\top & \mathbf{0}_{m \times n} \\ \mathbf{0}_{n \times m} & \mathbb{I}_n - vv^\top \end{bmatrix} \end{split}$$

So

$$\begin{split} P_B^{\perp} K &= \begin{bmatrix} \mathbb{I}_m - uu^{\top} & \mathbf{0}_{m \times n} \\ \mathbf{0}_{n \times m} & \mathbb{I}_n - vv^{\top} \end{bmatrix} \begin{bmatrix} \sigma \mathbb{I}_m & -A \\ -A^{\top} & \sigma \mathbb{I}_n \end{bmatrix} \\ &= \begin{bmatrix} \sigma(\mathbb{I}_m - uu^{\top}) & -A + \sigma uv^{\top} \\ -A^{\top} + \sigma vu^{\top} & \sigma(\mathbb{I}_n - vv^{\top}) \end{bmatrix} \\ &= K - \sigma \begin{bmatrix} uu^{\top} & -uv^{\top} \\ -vu^{\top} & \sigma vv^{\top} \end{bmatrix} \\ &= K - \sigma zz^{\top} \qquad z = \begin{bmatrix} u \\ -v \end{bmatrix} \end{split}$$

In particular, we see that effectively this is a low rank update of the original matrix! We can use the inversion formula for 2×2 block matrices, combined with the inverse of rank-1 update formulas:

$$\beta \coloneqq 1 - \sigma z^{\mathsf{T}} K^{\mathsf{+}} z = ?[\dots \text{ proof } \dots] = 0$$

Also $z \in \text{Im}(K)$, so, in particular, the case (vi) of the paper Generalized Inversion of Modified Matrices holds:

$$(A + cd^T)^{\dagger} = A^{\dagger} - kk^{\dagger}A^{\dagger} - A^{\dagger}h^{\dagger}h + (k^{\dagger}A^{\dagger}h^{\dagger})kh$$
 with $k = A^{\dagger}c, h = d^{\top}A^{\dagger}$

Assuming A is symmetric, c=d=x and noting that $v^*=\frac{1}{\|v\|^2}v^\top$ we can simplify since

$$k = h^{\top} = A^{+}x$$
 $k^{+} = \frac{1}{\|A^{+}x\|^{2}}x^{\top}A^{+}$ $h = k^{\top} = x^{\top}A^{+}$ $h^{+} = \frac{1}{\|A^{+}x\|^{2}}A^{+}x$

$$(A + xx^T)^{+} = A^{+} - \frac{A^{+}xx^{\top}A^{+}A^{+}}{\|A^{+}x\|^{2}} - \frac{A^{+}A^{+}xx^{\top}A^{+}}{\|A^{+}x\|^{2}} + \frac{(x^{\top}(A^{+})^{3}x)A^{+}xx^{\top}A^{+}}{\|A^{+}x\|^{4}}$$

With an additional scalar γ :

$$(A + \gamma x x^{T})^{+} = A^{+} - \frac{A^{+} x x^{\top} A^{+} A^{+}}{\|A^{+} x\|^{2}} - \frac{A^{+} A^{+} x x^{\top} A^{+}}{\|A^{+} x\|^{2}} + \frac{(x^{\top} (A^{+})^{3} x) A^{+} x x^{\top} A^{+}}{\|A^{+} x\|^{4}}$$

Now, in our case x happens to be an eigenvector: $Kz=2\sigma z,\ K^+z=\frac{1}{2\sigma}z,$ $\|z\|^2=2,$ hence $\|K^+z\|^2=\frac{1}{2\sigma^2}$ and $K^+zz^\top K^+=\frac{1}{4\sigma^2}zz^\top.$

$$\begin{split} (K - \sigma z z^T)^+ &= K^+ - \tfrac{1/(2\sigma)^3}{1/2\sigma^2} z z^\top - \tfrac{1/(2\sigma)^3}{1/2\sigma^2} z z^\top + \tfrac{2/(2\sigma)^3}{1/2\sigma^2} \tfrac{1/(2\sigma)^2}{1/2\sigma^2} z z^\top \\ &= K^+ - \tfrac{1}{4\sigma} z z^\top - \tfrac{1}{4\sigma} z z^\top + \tfrac{1}{4\sigma} z z^\top \\ &= K^+ - \tfrac{1}{4\sigma} z z^\top \end{split}$$

$$\implies (A + xx^T)^{+} =$$

Note that $v^* = \frac{1}{\|v\|^2} v^\top$.

3 The VJP

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

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

Now, we compute the terms individually:

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

And for the second term we get

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

Using the formula for inverting a 2×2 block-matrix, we can give an explicit solution to $K^{-\top} \begin{bmatrix} \phi \\ \psi \end{bmatrix}$:

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

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:

$$K \begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} \phi \\ \psi \end{bmatrix} \iff \begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} \sigma(\sigma^2 \mathbb{I}_m - AA^\top)^{-1} & (\sigma^2 \mathbb{I}_m - AA^\top)^{-1}A \\ (\sigma^2 \mathbb{I}_n - A^\top A)^{-1}A^\top & \sigma(\sigma^2 \mathbb{I}_n - A^\top A)^{-1} \end{bmatrix} \begin{bmatrix} \phi \\ \psi \end{bmatrix}$$

In particular, we can find the solution by solving 4 smaller linear systems:

$$\sigma(\sigma^{2}\mathbb{I}_{m} - AA^{\top})^{-1}\phi = x \qquad (\sigma^{2}\mathbb{I}_{m} - AA^{\top})^{-1}A\psi = y$$
$$(\sigma^{2}\mathbb{I}_{n} - A^{\top}A)^{-1}A^{\top}\phi = w \qquad \sigma(\sigma^{2}\mathbb{I}_{n} - A^{\top}A)^{-1}\psi = z$$

Or, equivalently:

$$(\sigma^{2}\mathbb{I}_{m} - AA^{\top})x = \sigma\phi \qquad (\sigma^{2}\mathbb{I}_{m} - AA^{\top})y = A\psi$$
$$(\sigma^{2}\mathbb{I}_{n} - A^{\top}A)w = A^{\top}\phi \qquad (\sigma^{2}\mathbb{I}_{n} - A^{\top}A)z = \sigma\psi$$

Note how this shows that the off-diagonal entries are solutions to regularized least squares problems! However, we really do not want to compute the matrices AA^{\top} and $A^{\top}A$ since this leads to numerical stability (squared condition number!) To circumvent this issue, we do a reformulation

$$(\sigma^{2}\mathbb{I}_{m} - AA^{\top})y = A\psi \iff y = \underset{y}{\operatorname{argmin}} \| - A^{\top}y - \psi \|_{2}^{2} - \sigma^{2}\|y\|_{2}^{2}$$

$$\iff y = \underset{y}{\operatorname{argmin}} \| \begin{bmatrix} A^{\top} \\ \sigma^{2}\mathbb{I}_{m} \end{bmatrix} y - \begin{bmatrix} -\psi \\ \mathbf{0}_{m} \end{bmatrix} \|_{2}^{2}$$

$$(\sigma^{2}\mathbb{I}_{n} - A^{\top}A)w = A^{\top}\phi \iff w = \underset{w}{\operatorname{argmin}} \|Aw + \phi\|_{2}^{2} - \sigma^{2}\|w\|_{2}^{2}$$

$$\iff w = \underset{w}{\operatorname{argmin}} \| \begin{bmatrix} A \\ \sigma^{2}\mathbb{I}_{n} \end{bmatrix} w - \begin{bmatrix} -\phi \\ \mathbf{0}_{n} \end{bmatrix} \|_{2}^{2}$$

Remark 1 (When is Ridge Regression unconstrained?). Consider the problem

$$\beta^* = \underset{\beta}{\operatorname{argmin}} \|X\beta - y\|^2 + \lambda \|\beta\|^2$$

Question: When is there an unconstrained solution? The solution satisfies the normal equation

$$(X^T X + \lambda \mathbb{I})\beta = X^\top y$$

If $\lambda>0$, then $(X^TX+\lambda\mathbb{I})$ is positive definite and hence invertible. If $\lambda<0$, then $(X^TX+\lambda\mathbb{I})$ is singular whenever λ is an eigenvalue of X^TX . In particular, the 4 systems listed before are all ill-conditioned! The central issue is that the constraint is missing! $\|u\|^2=1$ and $\|v\|^2=1$ translate to $u\perp\Delta u$ and $v\perp\Delta v$. Since u,v are singular vectors, this means we avoid the singular subspace when solving these equations!

What we should do is use **Riemannian Optimization**.

3.1 What happens if ϕ or ψ are zero?

In this case we want to fast track the calculation, meaning skip half of the necessary inversions. Looking at the equations we find that if $\phi=0$ then x=0 and w=0, and if $\psi=0$ then y=0 and z=0. This suggests that backward substitution is better than forward substitution, since it allows decoupling of the two gradient contributions.

3.2 Via Forward Substitution

Now, the diagonal entries we have a problem: the RHS lacks the A matrix. Thus, we solve in two steps instead:

$$\begin{split} A\mu &= \sigma \phi \implies x = \underset{x}{\operatorname{argmin}} \left\| \begin{bmatrix} A^\top \\ \sigma^2 \mathbb{I}_m \end{bmatrix} x - \begin{bmatrix} -\mu \\ \mathbf{0}_m \end{bmatrix} \right\|_2^2 \\ A^\top \nu &= \sigma \psi \implies z = \underset{z}{\operatorname{argmin}} \left\| \begin{bmatrix} A \\ \sigma^2 \mathbb{I}_n \end{bmatrix} z - \begin{bmatrix} -\nu \\ \mathbf{0}_n \end{bmatrix} \right\|_2^2 \end{split}$$

We can optimize further by performing a simultaneous solve:

$$\begin{bmatrix} x, y \end{bmatrix} = \underset{x,y}{\operatorname{argmin}} \left\| \begin{bmatrix} A^{\top} \\ \sigma^{2} \mathbb{I}_{m} \end{bmatrix} \begin{bmatrix} x, y \end{bmatrix} - \begin{bmatrix} -\mu & -\psi \\ \mathbf{0}_{m} & \mathbf{0}_{m} \end{bmatrix} \right\|_{2}^{2} \quad \mu = \underset{\mu}{\operatorname{argmin}} \|A\mu - \sigma\phi\|_{2}^{2}$$

$$[w, z] = \underset{w,z}{\operatorname{argmin}} \left\| \begin{bmatrix} A \\ \sigma^{2} \mathbb{I}_{n} \end{bmatrix} [w, z] - \begin{bmatrix} -\phi & -\nu \\ \mathbf{0}_{n} & \mathbf{0}_{n} \end{bmatrix} \right\|_{2}^{2} \quad \nu = \underset{\nu}{\operatorname{argmin}} \|A^{\top}\nu - \sigma\psi\|_{2}^{2}$$

3.3 Via Backward Substitution

We need to introduce an additional modification:

If $A\mu = \sigma\phi$ not solveable, we instead can multiply the equation by A^{\top} to obtain:

$$(\sigma^{2}\mathbb{I}_{m} - AA^{\top})x = \sigma\phi \qquad \Longrightarrow \qquad (\sigma^{2}\mathbb{I}_{n} - A^{\top}A)\mu = \sigma A^{\top}\phi \qquad A^{\top}x = \mu$$
$$(\sigma^{2}\mathbb{I}_{n} - A^{\top}A)z = \sigma\psi \qquad \Longrightarrow \qquad (\sigma^{2}\mathbb{I}_{n} - A^{\top}A)A\nu = \sigma A\psi \qquad Az = \nu$$

So:

$$\mu = \underset{\mu}{\operatorname{argmin}} \left\| \begin{bmatrix} A \\ \sigma^{2} \mathbb{I}_{n} \end{bmatrix} \mu - \begin{bmatrix} -\sigma \phi \\ \mathbf{0}_{n} \end{bmatrix} \right\|_{2}^{2} \qquad A^{\top} x = \mu$$

$$\nu = \underset{\mu}{\operatorname{argmin}} \left\| \begin{bmatrix} A^{\top} \\ \sigma^{2} \mathbb{I}_{m} \end{bmatrix} \nu - \begin{bmatrix} -\sigma \psi \\ \mathbf{0}_{m} \end{bmatrix} \right\|_{2}^{2} \qquad Az = \nu$$

So

$$\begin{bmatrix} \mu & w \end{bmatrix} = \begin{bmatrix} A \\ \sigma^2 \mathbb{I}_n \end{bmatrix} \begin{bmatrix} -\sigma \phi & -\phi \\ \mathbf{0}_n & \mathbf{0}_n \end{bmatrix}$$

$$\begin{bmatrix} y & \nu \end{bmatrix} = \begin{bmatrix} A^\top \\ \sigma^2 \mathbb{I}_m \end{bmatrix} \begin{bmatrix} -\psi & -\sigma \psi \\ \mathbf{0}_m & \mathbf{0}_m \end{bmatrix}$$

In principle, one could try to rephrase these as smaller problems, but for now, it's better to just stick to the bigger system. We can use the **push-through** identity to convert these into 4 linear systems:

$$\begin{aligned} Px &= \phi & Py &= \tilde{A}\psi \\ Qz &= \tilde{A}^\top \phi & Qw &= \psi \end{aligned}$$

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

$$\xi^{\top} \frac{\partial \sigma}{\partial A} = \xi u v^{\top}$$

$$\phi^{\top} \frac{\partial u}{\partial A} = (\mathbb{I}_m - u u^{\top}) \tilde{\phi} v^{\top} = (\tilde{\phi} - (u^{\top} \tilde{\phi}) u) v^{\top}$$

$$\psi^{\top} \frac{\partial v}{\partial A} = u \tilde{\psi}^{\top} (\mathbb{I}_n - v v^{\top}) = u (\tilde{\psi} - (v^{\top} \tilde{\psi}) v)^{\top}$$

4 Spectral Normalization

The VJP of spectral normalization can be computed as follows: let $g(A) = ||A||_2$ and V be the vector in the VJP. then

$$\begin{split} \nabla_A \langle V \mid \frac{A}{\|A\|_2} \rangle &= \langle V | \frac{A + \Delta A}{g(A + \Delta A)} - \frac{A}{g(A)} \rangle \\ &= \langle V | \frac{A + \Delta A}{g(A) + \nabla g(A) \Delta A} - \frac{A}{g(A)} \rangle \\ &= \langle V | \frac{(A + \Delta A)(g(A) - \nabla g(A) \Delta A)}{(g(A) + \nabla g(A) \Delta A)(g(A) - \nabla g(A) \Delta A)} - \frac{A}{g(A)} \rangle \\ &= \langle V | \frac{\Delta A g(A) - A \nabla g(A) \Delta A}{g(A)^2} \rangle \\ &= \langle \frac{1}{g(A)} V - \frac{\langle V | A \rangle}{g(A)} \nabla g(A) | \Delta A \rangle \end{split}$$

$$g(A) = 1 \implies \nabla_A \langle V \mid \frac{A}{\|A\|_2} \rangle = \langle V - \langle V \mid A \rangle \nabla g(A) \mid \Delta A \rangle$$

5 Projected gradient

When using spectral normalization we want to do the following:

update:
$$A' = A - \nabla_A \mathcal{L}(\frac{A}{\|A\|_2})$$

project: $A = \frac{A'}{\|A'\|_2}$

Moreover, we want:

- \bullet During forward, compute $\frac{A}{\|A\|_2}$ only once and then reuse this node.
- Compute $||A||_2$ effectively between gradient updates.
 - Avoid built-in torch algos, as they make use of full SVD algos.
- After gradient update, perform projection step. (maybe unnecessary)

NOTE: gradients are different if we include normalization!