THE SINGULAR VALUE DECOMPOSITION (Cont.)

- **The Pseudo-inverse**
- **Use of SVD for least-squares problems**
- **Application to regularization**
- **Numerical rank**

Pseudo-inverse of an arbitrary matrix

➤ Let $A = U\Sigma V^T$ which we rewrite as

$$A = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} = U_1 \Sigma_1 V_1^T$$

➤ Then the pseudo inverse of A is:

$$A^\dagger = V_1 \Sigma_1^{-1} U_1^T = \sum_{j=1}^{r} \frac{1}{\sigma_j} v_j u_j^T$$

➤ The pseudo-inverse of A is the mapping from a vector b to the (unique) Minumum Norm solution of the LS problem: $\min_x \|Ax - b\|_2^2$ – (to be shown)

➤ In the full-rank overdetermined case, the normal equations yield $x = \underbrace{(A^TA)^{-1}A^T}_{A^\dagger} b$

Least-squares problem via the SVD

Problem: $\min_x \|b - Ax\|_2$ in general case.

➤ We want to:

- Find *all* possible least-squares solutions.
- Also find the one with min. 2-norm.

➤ SVD of A will play instrumental role in expressing solution

➤ Write SVD of A as:

$$\boxed{A = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^T \\ V_2^T \end{pmatrix} = \sum_{i=1}^{r} \sigma_i v_i u_i^T}$$

1) Express x in V basis : $x = Vy = [V_1, \ V_2] \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$

2) Then left multiply by U^T to get

$$\|Ax - b\|_2^2 = \left\| \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} - \begin{pmatrix} U_1^T b \\ U_2^T b \end{pmatrix} \right\|_2^2$$

3) Find all possible solutions in terms of $y = [y_1; y_2]$

1 What are **all** least-squares solutions to the above system? Among these which one has minimum norm?

Answer: From above, must have $y_1 = \Sigma_1^{-1} U_1^T b$ and $y_2 =$ anything (free).

Recall that:
$$x = [V_1, V_2] \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = V_1 y_1 + V_2 y_2$$
$$= V_1 \Sigma_1^{-1} U_1^T b + V_2 y_2$$
$$= \boxed{A^\dagger b + V_2 y_2}$$

➤ Note: $A^\dagger b \in \mathbf{Ran}(A^T)$ and $V_2 y_2 \in \mathbf{Null}(A)$.

➤ Therefore: least-squares solutions are all of the form:

$$A^\dagger b + w \quad \text{where} \quad w \in \mathbf{Null}(A).$$

➤ Smallest norm when $y_2 = 0$, i.e., when $w = 0$.

➤ Minimum norm solution to $\min_x \|Ax - b\|_2^2$ satisfies $\Sigma_1 y_1 = U_1^T b$, $y_2 = 0$.

➤ It is:
$$x_{LS} = V_1 \Sigma_1^{-1} U_1^T b = A^\dagger b$$

✍2 If $A \in \mathbb{R}^{m\times n}$ what are the dimensions of $A^\dagger$?, $A^\dagger A$?, $AA^\dagger$?

✍3 Show that $A^\dagger A$ is an orthogonal projector. What are its range and null-space?

✍4 Same questions for $AA^\dagger$.

Moore-Penrose Inverse

The pseudo-inverse of A is given by

$$A^\dagger = V \begin{pmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0 \end{pmatrix} U^T = \sum_{i=1}^{r} \frac{v_i u_i^T}{\sigma_i}$$

Moore-Penrose conditions:

The pseudo inverse X of a matrix is uniquely determined by these four conditions:

(1) $AXA = A$ (2) $XAX = X$

(3) $(AX)^H = AX$ (4) $(XA)^H = XA$

➤ In the full-rank overdetermined case, $A^\dagger = (A^T A)^{-1} A^T$

Least-squares problems and the SVD

➤ The SVD can give much information on solutions of overdetermined and underdetermined linear systems.

Let A be an $m \times n$ matrix and $A = U\Sigma V^T$ its SVD with $r = \mathbf{rank}(A)$, $V = [v_1, \ldots, v_n]$ $U = [u_1, \ldots, u_m]$. Then

$$x_{LS} = \sum_{i=1}^{r} \frac{u_i^T b}{\sigma_i} v_i$$

minimizes $\|b - Ax\|_2$ and has the smallest 2-norm among all possible minimizers. In addition,

$$\rho_{LS} \equiv \|b - Ax_{LS}\|_2 = \|z\|_2 \text{ with } z = [u_{r+1}, \ldots, u_m]^T b$$

Least-squares problems and pseudo-inverses

➤ A restatement of the first part of the previous result:

Consider the general linear least-squares problem

$$\min_{x \in S} \|x\|_2, \quad S = \{x \in \mathbb{R}^n \mid \|b - Ax\|_2 \min\}.$$

This problem always has a unique solution given by

$$x = A^\dagger b$$

✍5 Consider the matrix:

$$A = \begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 0 & -2 & 1 \end{pmatrix}$$

- Compute the thin SVD of A
- Find the matrix B of rank 1 which is the closest to the above matrix in the 2-norm sense.
- What is the pseudo-inverse of A?
- What is the pseudo-inverse of B?
- Find the vector x of smallest norm which minimizes $\|b - Ax\|_2$ with $b = (1, 1)^T$
- Find the vector x of smallest norm which minimizes $\|b - Bx\|_2$ with $b = (1, 1)^T$

Ill-conditioned systems and the SVD

➤ Let A be $m \times m$ and $A = U\Sigma V^T$ its SVD

➤ Solution of $Ax = b$ is $x = A^{-1}b = \sum_{i=1}^m \frac{u_i^T b}{\sigma_i} v_i$

➤ When A is very ill-conditioned, it has many small singular values. The division by these small σ_i's will amplify any noise in the data. If $\tilde{b} = b + \epsilon$ then

$$A^{-1}\tilde{b} = \sum_{i=1}^m \frac{u_i^T b}{\sigma_i} v_i + \underbrace{\sum_{i=1}^m \frac{u_i^T \epsilon}{\sigma_i} v_i}_{Error}$$

➤ Result: solution could be completely meaningless.

Remedy: SVD regularization

Truncate the SVD by only keeping the $\sigma_i's$ that are $\geq \tau$, where τ is a threshold

➤ Gives the Truncated SVD solution (TSVD solution:)

$$x_{TSVD} = \sum_{\sigma_i \geq \tau} \frac{u_i^T b}{\sigma_i} v_i$$

➤ Many applications [e.g., Image and signal processing,..]

Numerical rank and the SVD

➤ Assuming the original matrix A is exactly of rank k the computed SVD of A will be the SVD of a nearby matrix $A + E$ – Can show: $|\hat{\sigma}_i - \sigma_i| \le \alpha\, \sigma_1 \underline{\mathbf{u}}$

➤ Result: zero singular values will yield small computed singular values and r larger sing. values.

➤ Reverse problem: *numerical rank* – The ϵ-rank of A :

$$r_\epsilon = \min\{rank(B) : B \in \mathbb{R}^{m\times n}, \|A - B\|_2 \le \epsilon\},$$

✍6 Show that r_ϵ equals the number sing. values that are $>\epsilon$

✍7 Show: r_ϵ equals the number of columns of A that are linearly independent for any perturbation of A with norm $\le \epsilon$.

➤ Practical problem : How to set ϵ?

Pseudo inverses of full-rank matrices

Case 1: $m \ge n$ Then $A^\dagger = (A^TA)^{-1}A^T$

➤ Thin SVD is $A = U_1\Sigma_1V_1^T$ and V_1, Σ_1 are $n \times n$. Then:

$$\begin{aligned}(A^TA)^{-1}A^T &= (V_1\Sigma_1^2V_1^T)^{-1}V_1\Sigma_1U_1^T\\ &= V_1\Sigma_1^{-2}V_1^TV_1\Sigma_1U_1^T\\ &= V_1\Sigma_1^{-1}U_1^T\\ &= A^\dagger\end{aligned}$$

Example: Pseudo-inverse of $\begin{pmatrix}0 & 1\\ 1 & 2\\ 2 & -1\\ 0 & 1\end{pmatrix}$ is?

Case 2: $m < n$ Then $A^\dagger = A^T(AA^T)^{-1}$

➤ Thin SVD is $A = U_1\Sigma_1V_1^T$. Now U_1, Σ_1 are $m \times m$ and:

$$\begin{aligned}A^T(AA^T)^{-1} &= V_1\Sigma_1U_1^T[U_1\Sigma_1^2U_1^T]^{-1}\\ &= V_1\Sigma_1U_1^TU_1\Sigma_1^{-2}U_1^T\\ &= V_1\Sigma_1\Sigma_1^{-2}U_1^T\\ &= V_1\Sigma_1^{-1}U_1^T\\ &= A^\dagger\end{aligned}$$

Example: Pseudo-inverse of $\begin{pmatrix}0 & 1 & 2 & 0\\ 1 & 2 & -1 & 1\end{pmatrix}$ is?

➤ Mnemonic: The pseudo inverse of A is A^T completed by the inverse of the smaller of $(A^TA)^{-1}$ or $(AA^T)^{-1}$ where it fits (i.e., left or right)