THE SINGULAR VALUE DECOMPOSITION

- The SVD – existence - properties.
- Pseudo-inverses and the SVD
- Use of SVD for least-squares problems
- Applications of the SVD
- Text: mainly sect. 2.4

The Singular Value Decomposition (SVD)

Theorem For any matrix $A \in \mathbb{R}^{m\times n}$ there exist unitary matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ such that

$$A = U\Sigma V^T$$

where Σ is a diagonal matrix with entries $\sigma_{ii} \geq 0$.

$$\sigma_{11} \geq \sigma_{22} \geq \cdots \sigma_{pp} \geq 0 \text{ with } p = \min(n, m)$$

- The σ_{ii} are the singular values of A.
- σ_{ii} is denoted simply by σ_i

Proof: Let $\sigma_1 = \|A\|_2 = \max_{x,\|x\|_2=1} \|Ax\|_2$. There exists a pair of unit vectors v_1, u_1 such that

$$Av_1 = \sigma_1 u_1$$

- Complete v_1 into an orthonormal basis of $\mathbb{R}^n$

$$V \equiv [v_1, V_2] = n \times n \text{ unitary}$$

- Complete u_1 into an orthonormal basis of $\mathbb{R}^m$

$$U \equiv [u_1, U_2] = m \times m \text{ unitary}$$

- Then, it is easy to show that

$$AV = U \times \begin{pmatrix} \sigma_1 & w^T \\ 0 & B \end{pmatrix} \rightarrow U^T AV = \begin{pmatrix} \sigma_1 & w^T \\ 0 & B \end{pmatrix} \equiv A_1$$

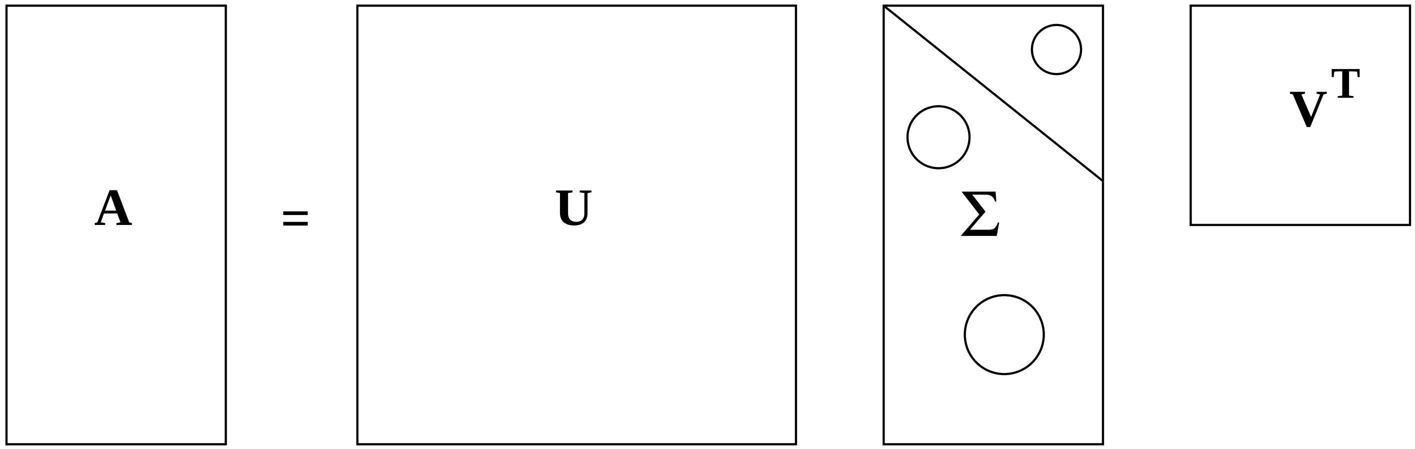
- Observe that

$$\left\| A_1 \begin{pmatrix} \sigma_1 \\ w \end{pmatrix} \right\|_2 \geq \sigma_1^2 + \|w\|^2 = \sqrt{\sigma_1^2 + \|w\|^2} \left\| \begin{pmatrix} \sigma_1 \\ w \end{pmatrix} \right\|_2$$

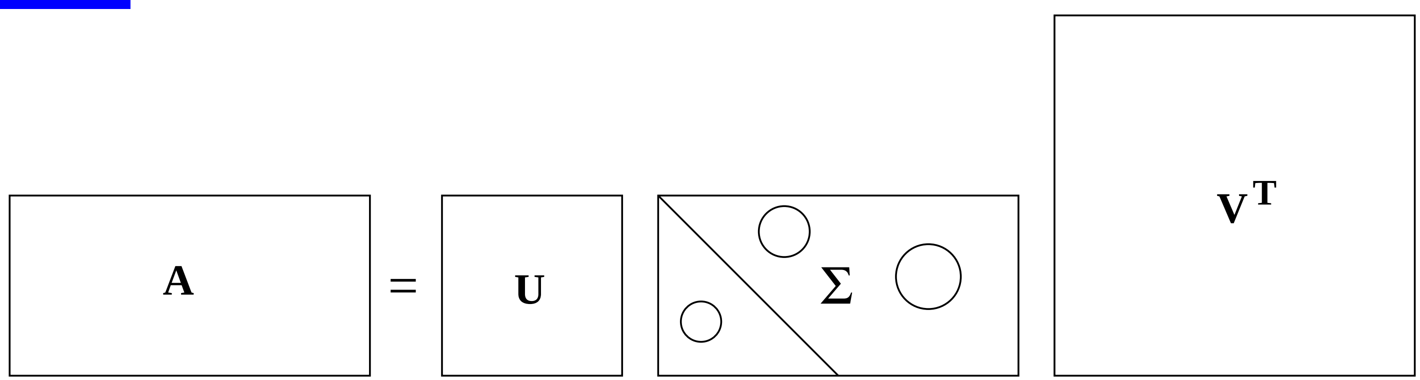
- This shows that w must be zero [why?]

- Complete the proof by an induction argument.

Case 1:



Case 2:



The “thin” SVD

➤ Consider the Case-1. It can be rewritten as

$$A = [U_1 U_2] \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} V^T$$

Which gives:

$$\boxed{A = U_1 \Sigma_1 V^T}$$

where U_1 is $m \times n$ (same shape as A), and Σ_1 and V are $n \times n$

➤ referred to as the “thin” SVD. Important in practice.

✍ How can you obtain the thin SVD from the QR factorization of A and the SVD of an $n \times n$ matrix?

A few properties. Assume that

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0 \text{ and } \sigma_{r+1} = \cdots = \sigma_p = 0$$

Then:

- $\text{rank}(A) = r$ = number of nonzero singular values.
- $\text{Ran}(A) = \text{span}\{u_1, u_2, \ldots, u_r\}$
- $\text{Null}(A) = \text{span}\{v_{r+1}, v_{r+2}, \ldots, v_n\}$
- The matrix A admits the SVD expansion:

$$A = \sum_{i=1}^{r} \sigma_i u_i v_i^T$$

Properties of the SVD (continued)

- $\|A\|_2 = \sigma_1$ = largest singular value
- $\|A\|_F = \left(\sum_{i=1}^r \sigma_i^2\right)^{1/2}$
- When A is an $n \times n$ nonsingular matrix then $\|A^{-1}\|_2 = 1/\sigma_n$ = inverse of smallest s.v.

Let $k < r$ and

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$$

then

$$\min_{rank(B)=k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}$$

Right and Left Singular vectors:

$$Av_i = \sigma_i u_i$$
$$A^T u_j = \sigma_j v_j$$

- Consequence $A^T A v_i = \sigma_i^2 v_i$ and $A A^T u_i = \sigma_i^2 u_i$
- Right singular vectors (v_i's) are eigenvectors of $A^T A$
- Left singular vectors (u_i's) are eigenvectors of $A A^T$
- Possible to get the SVD from eigenvectors of AA^T and $A^T A$ – but: difficulties due to non-uniqueness of the SVD

Define the $r \times r$ matrix

$$\Sigma_1 = \mathrm{diag}(\sigma_1, \ldots, \sigma_r)$$

- Let $A \in \mathbb{R}^{m\times n}$ and consider A^TA ($\in \mathbb{R}^{n\times n}$):

$$A^TA = V\Sigma^T\Sigma V^T \;\rightarrow\; A^TA = V \underbrace{\begin{pmatrix} \Sigma_1^2 & 0 \\ 0 & 0 \end{pmatrix}}_{n\times n} V^T$$

- This gives the spectral decomposition of A^TA.

➤ **Similarly, U gives the eigenvectors of AA^T.**

$$AA^T = U \underbrace{\begin{pmatrix} \Sigma_1^2 & 0 \\ 0 & 0 \end{pmatrix}}_{m \times m} U^T$$

Important:

$A^TA = VD_1V^T$ **and** $AA^T = UD_2U^T$ **give the SVD factors** U, V **up to signs!**

Pseudo-inverse of an arbitrary matrix

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 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, $A^{\dagger} = (A^T A)^{-1} A^T$

➤ **SVD can give much information about solving overdetermined and underdetermined linear systems.**

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

$$x = A^{\dagger} b$$

✍ Consider the matrix:

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

- Compute the singular value decomposition 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 $\geq \tau$, 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 processing,..]

Numerical rank and the SVD

- Assume that the original matrix A is exactly of rank k.
- The computed SVD of A will be the SVD of a nearby matrix $A + E$.
- Easy to show that $|\hat{\sigma}_i - \sigma_i| \leq \alpha\ \sigma_1 \underline{\mathbf{u}}$
- Result: zero singular values will yield small computed singular values
- Determining the "numerical rank:" treat singular values below a certain threshold δ as zero.
- Practical problem : need to set δ.