

Singular Value Decomposition

Strang's discussion had to be rearranged and extended so it made sense.

Thm SVD: General matrix  $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$

Here e.g.  $n < m$

$$\begin{bmatrix} n \\ m \end{bmatrix}$$

$$A = Q_1 \Sigma Q_2^T$$

where

$Q_1$  O.N. - cols are EVs of  $A^T A$

$Q_2$  O.N. - " " " " "  $A A^T$

$$\Sigma = \begin{bmatrix} \Delta & 0 \\ 0 & 0 \end{bmatrix} \quad \Delta = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{bmatrix}$$

$r = \text{rank}(A)$

For  $i = 1, \dots, r$   $\lambda_i$  is pos EW of both  $A^T A$  &  $A A^T$

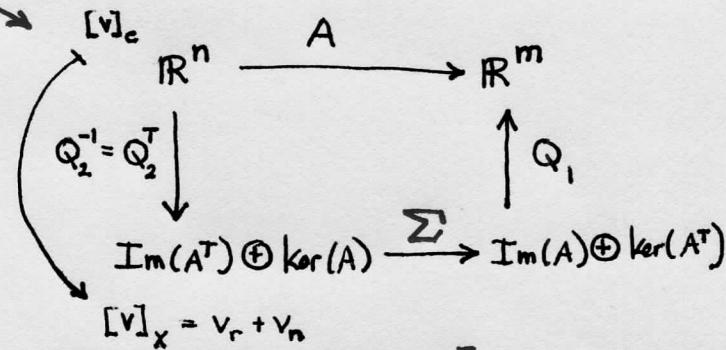
Define  $\sigma_i = \sqrt{\lambda_i}$

$$A \text{ Complex} \Rightarrow A = U_1 \Sigma U_2^H$$

unitary

Key ideas which will become clearer as we proceed:

$$A = Q_1 \Sigma Q_2^T = \begin{bmatrix} 1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -x_1^T \\ \vdots \\ -x_r^T \\ 0 \end{bmatrix}$$



Change of basis matrix  $Q_2^T$  takes a co-ord vector  $[v]_e$  in orig basis to a new co-ord vector in terms of the basis  $\{x_1, \dots, x_r, x_{r+1}, \dots, x_n\}$

Spectral Thm

$\exists$  a full set of O.N. EVs  $x_j$ :

$$A^T A x_j = \lambda_j x_j \quad \text{and}$$

$$x_j^T x_k = 0 \quad \text{if } j \neq k$$

$$\text{Put these in cols of } Q_2 = \begin{bmatrix} 1 & | & x_1 & \dots & x_n \\ | & | & | & \dots & | \end{bmatrix}$$

Now observe that all  $\lambda_j$  are in fact non-neg:  $x_j^T A^T A x_j = x_j^T \lambda_j x_j$

$$(A x_j)^T A x_j = \lambda_j$$

$$0 \leq \|A x_j\|_2^2 = \lambda_j$$

Let's order these so  $\lambda_1, \dots, \lambda_r$  are pos and  $\lambda_j = 0$  for  $j = r+1, \dots, n$

Then  $A x_j = 0$  for  $j = r+1, \dots, n$  i.e.  $A x_j = 0 x_j$

This tells us  $r = \text{rank}(A)$  because we show  $\dim(\ker(A)) = n-r$  [rank-nullity Thm]

Lemma:  $\ker(A) = \text{Span}\{x_{r+1}, \dots, x_n\}$

Pf. by contrad.: Suppose there was  $v \in \text{Span}\{x_1, \dots, x_r\} \ni Av = 0$ .  $v = \sum_1^r \alpha_i x_i$  and some  $\alpha_i \neq 0$

$$\text{Then } A^T(Av) = A^T 0 = 0 \Rightarrow (A^T A)(v) = (A^T A)(\sum \alpha_i x_i) = 0$$

$$\sum \alpha_i (A^T A x_i) = \sum \alpha_i \lambda_i x_i = 0$$

but  $\lambda_i > 0$  and  $\sum x_i$  is LI  $\Rightarrow$  each  $\alpha_i = 0$

Confd  $\rightarrow$

Step 2 Define cols of  $Q_1$

For  $i=1, \dots, r$  define  $\sigma_j = \sqrt{\lambda_j}$  the "singular values"  
 $q_j = \frac{1}{\sigma_j} Ax_j \implies Ax_j = \sigma_j q_j$  key relation

We see  $\{q_j\}$  is ON:

$$q_i^T q_j = \frac{1}{\sigma_i} \frac{1}{\sigma_j} (x_i^T A^T A x_j) = \frac{\lambda_j}{\sigma_i \sigma_j} x_i^T x_j = \begin{cases} 0 & i \neq j \\ \frac{\lambda_j}{\sigma_j^2} = 1 & i = j \end{cases}$$

Extend  $\{q_1, \dots, q_r\}$  using Gram-Schmidt to add ON  $\{q_{r+1}, \dots, q_m\}$

$$Q_1 := \begin{bmatrix} | & | & | \\ q_1 & \dots & q_r \\ | & | & | \end{bmatrix}$$

Step 3 Now define  $\Sigma := Q_1^T A Q_2$

$$\text{Elt } \Sigma_{ij} = (Q_1^T A Q_2)_{ij} = q_i^T A x_j = \begin{cases} q_i^T \sigma_j q_j & \text{if } j \leq r \text{ because } Ax_j = \sigma_j q_j \\ 0 & \text{if } j > r \text{ because } Ax_j = \lambda_j x_j = 0 x_j = 0 \end{cases}$$

BUT  $q_i^T q_j = 0$  for  $i \neq j$   
so we really get  $\begin{cases} \sigma_i & i=j \\ 0 & i \neq j \end{cases}$

$$\begin{bmatrix} -q_i^T - \\ - \end{bmatrix} \begin{bmatrix} Ax_j \\ 1 \end{bmatrix}$$

The only nonzero elts in  $\Sigma$

are  $\Sigma_{ii} = \sigma_i$  for  $i=1, \dots, r$

► so  $\Sigma = Q_1^T A Q_2 \implies A = Q_1 \Sigma Q_2^T$  QED

COR 1.  $\{x_1, \dots, x_r\}$  is ON basis for RowSpace(A) = Col(A<sup>T</sup>) = Im(A<sup>T</sup>)

2.  $\{x_{r+1}, \dots, x_n\}$  ON basis  $\ker(A)$

3.  $\{q_1, \dots, q_r\}$  ON basis  $\text{Col}(A) = \text{Im}(A) = A(\mathbb{R}^n)$

4.  $\{q_{r+1}, \dots, q_m\}$  ON basis  $\ker(A^T)$

(2) we proved as Lemma in Step 1

(1) follows from Strang's Fund Thm LA II :  $\mathbb{R}^n = \overbrace{\text{Im}(A^T)}^{\ker(A)^{\perp}} \oplus \ker(A)$

(3) choose any  $w \in \text{Col}(A)$ . we must show it can be expressed as LC  $\{q_1, \dots, q_r\}$

By def  $\exists u \in \mathbb{R}^n \ni Au = w$

By Step 1 Lemma  $u = \sum \alpha_i x_i$  thus  $Au = A(\sum \alpha_i x_i) = \sum \alpha_i Ax_i \stackrel{\substack{\text{step 2 key relation} \\ \downarrow}}{=} \sum \alpha_i \sigma_i q_i$   
so  $w = \text{LC } \{q_1, \dots, q_r\}$

(4) Since  $\mathbb{R}^n = \text{Im}(A) \oplus \underbrace{\ker(A^T)}_{\text{Im}(A)^{\perp}}$  we see  $\{q_{r+1}, \dots, q_m\}$  must span  $\ker(A^T)$

□

(3)

Strang gives some remarks:

① For  $A$  symm pos def, SVD is just  $A = Q \Lambda Q^T$

$$Q_1 = \begin{bmatrix} | & | & | & | \\ | & \dots & | & | \end{bmatrix}_{\substack{r \\ \text{col}(A) \\ m-r \\ \text{ker}(A^T)}} \quad Q_2 = \begin{bmatrix} | & | & | & | \\ | & \dots & | & | \end{bmatrix}_{\substack{r \\ \text{col}(A^T) \\ n-r \\ \text{ker}(A)}}$$

③  $A Q_2 = Q_1 \Sigma$  i.e.  $Ax_j = \sigma_j q_j$  where  $\sigma_j = 0$  if  $j > r$

④ By construction in the pf,  $Q_2 = [x_1 \dots x_n]$  is EV matrix of  $A^T A$  w/ EWS  $\lambda_i$ . What about  $AA^T$ ?  $AA^T = Q_1 \Sigma Q_2^T Q_2 \Sigma^T Q_1^T = Q_1 \Sigma \Sigma^T Q_1^T \Rightarrow (AA^T)Q_1 = Q_1(\Sigma \Sigma^T)$

Using my block multiplying notation in ch 2 sheets  $B_k^{\ell} \leftarrow \text{cols}$   $(B_k^{\ell})^T = B_{\ell}^k$

$$\begin{aligned} \text{Let } r+k &= n \\ r+\ell &= m \end{aligned}$$

$$\begin{bmatrix} \Delta_r^r & 0_r^k \\ 0_r^r & 0_r^k \end{bmatrix}_{\Sigma} \begin{bmatrix} \Delta_r^r & 0_r^{\ell} \\ 0_k^r & 0_k^{\ell} \end{bmatrix}_{\Sigma^T} = \begin{bmatrix} \Delta_r^r \Delta_r^r + 0_r^k 0_k^r & \Delta_r^r 0_r^{\ell} + 0_r^k 0_k^{\ell} \\ 0_k^r \Delta_r^r + 0_r^k 0_k^r & 0_k^r 0_r^{\ell} + 0_k^k 0_k^{\ell} \end{bmatrix}$$

$$= \begin{bmatrix} (\Delta^2)_r^r & 0_r^{\ell} \\ 0_r^r & 0_r^{\ell} \end{bmatrix} \quad \Delta^2 = \begin{bmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_r^2 \end{bmatrix} = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_r \end{bmatrix}$$

$$m \begin{bmatrix} A \\ A^T \end{bmatrix} \begin{bmatrix} Q_1 \end{bmatrix} = \begin{bmatrix} 1 & | & | & | \\ | & \dots & | & | \\ | & \dots & | & | \\ | & \dots & | & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & 0 \end{bmatrix}$$

⑤ For a numerically stable def of  $\text{rank}(A)$ , we can't count pivots, so we count the non-zero  $\sigma_i$  values [ $A^T A$  has EWS  $\sigma_i^2$ ] we decree  $\sigma_i = 0$  if say  $\sigma_i < 10^{-6}$ . EFFECTIVE RANK

### Polar Decomposition

$$\begin{array}{ccc} \mathbb{R}^n & \xrightarrow{A} & \mathbb{R}^m \\ Q_2^T \downarrow & & \uparrow Q_1 \\ \text{Im}(A^T) \oplus \text{ker}(A) & \xrightarrow{\Sigma} & \text{Im}(A) \oplus \text{ker}(A^T) \end{array}$$

We can see how the action of any matrix is broken up into rotation/reflection  $Q_2, Q_1$  and stretching/compressing  $\Sigma$

Thm  $A$   $n \times n$  square, Real  $\Rightarrow A = QS$

$$Q = O.N$$

S = Symm, pos semidef

[ $A$  nsing  $\Rightarrow S$  pos def]

$$\begin{aligned} \text{Pf. } A &= Q_1 \Sigma Q_2^T \\ &= Q_1 (Q_2^T Q_2) \Sigma Q_2^T \\ &= \underbrace{(Q_1 Q_2^T)}_Q \underbrace{(\Sigma Q_2^T)}_S \end{aligned}$$

ON rotation, reflection      Stretching

□

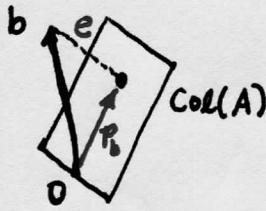
## Least Squares and SVD

From ch 3.3 we want to solve  $Ax = b$  for  $A: \mathbb{R}^n \rightarrow \mathbb{R}^m$

$$m \begin{bmatrix} n \\ A \end{bmatrix} \begin{bmatrix} x \end{bmatrix}^n = \begin{bmatrix} b \end{bmatrix}^m$$

- 3 Things can go wrong in general
- 1) Sys of eqs inconsistent,  $b \notin \text{Col}(A)$
  - 2) Rows of  $A$  are LD (must happen if  $m > n$ )
  - 3) Cols of  $A$  are LD  $\leftarrow$  This was not encountered in ch 3.3

Let's recap what we did in ch 3.3:



We OG proj  $b$  into  $\text{Col}(A)$  and get  $P_b$  and by def of  $\text{Col}(A)$

There must be some  $\bar{x} \ni A\bar{x} = P_b$ .  $e := b - A\bar{x}$

$e \in \ker(A^T)$  because  $\mathbb{R}^m = \text{Col}(A) \oplus \ker(A^T)$

Then  $A^T e = 0 \Rightarrow A^T(b - A\bar{x}) = 0 \Rightarrow A^T A \bar{x} = A^T b$

We showed if  $A$  has LI cols,  $A^T A$  is invertible and  $\bar{x} = (A^T A)^{-1} A^T b$

That took care of cases (1) and (2). Now we must also handle (3) cols of  $A$  not LI:

If cols of  $A$  are LD  $\Rightarrow \ker(A) \neq \{0\}$  so  $A^T A \bar{x}$  is not one-to-one

$\mathbb{R}^n = \text{Col}(A^T) \oplus \ker(A)$  so  $\bar{x} = x_p + x_n$ . Any  $x_n \in \ker(A)$  gives same value for  $A^T A(x_p + x_n)$

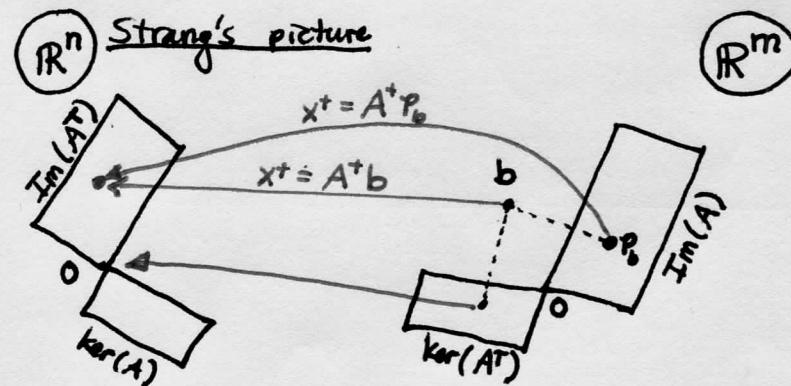
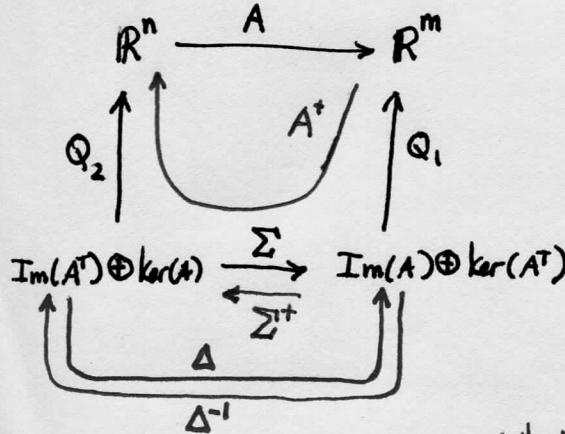
Key Idea: choose  $\bar{x}$  of minimum length [i.e.  $x_n = 0$ ]. Then  $\bar{x} = x_p = x^+$

Thm the minimum length soln to  $Ax = b$  is  $x^+ = A^+ b$ , where we use the SVD to find the 'Generalized inverse'  $A^+ := Q_2 \Sigma^+ Q_1^T$

$$\text{and from } \Sigma = \begin{bmatrix} \Delta & 0 \\ 0 & 0 \end{bmatrix} \quad \Delta = \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{bmatrix}$$

$$\text{we get } \Sigma^+ := \begin{bmatrix} \Delta^{-1} & 0 \\ 0 & 0 \end{bmatrix} \quad \begin{array}{l} 1. \text{ Transpose} \\ 2. \text{ Take reciprocals in } \Delta \end{array}$$

We need a warm-up example and a Lemma before giving the pf, but first a picture of what is going on:



What is the relationship between  $A^T$  and  $A^{-1}$ ?

For  $A^{-1}$  to exist, we need  $n=m$  and  $\ker(A) = \{0\} \Rightarrow$  then  $\Sigma = \Delta$

But  $A^T = A^{-1}$  only if  $A = Q$  a O.N. matrix

because only then is  $\Delta = I$  no stretching in any direction.

cont'd

warm-up example

$$A = \Sigma = \begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

Here  $A: \mathbb{R}^4 \rightarrow \mathbb{R}^3$

usually we think of  $m > n$   
but here we don't just to  
show it works in all cases.

We are showing  $\sum x = b$  has soln  $x^+ = \Sigma^+ b$

$\text{Col}(A) = \{(y_1, y_2, 0)\}$  so  $\text{Proj}(b) = \begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix}$  and what  $\bar{x}$  would map to this?

We can see

$$\begin{bmatrix} \sigma_1 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ \frac{b_1}{\sigma_1} \\ b_2 \\ \frac{b_2}{\sigma_2} \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ 0 \end{bmatrix}$$

so  $x_3$  and  $x_4$  are arb  
and  $\bar{x}$  is not unique.

We choose  $x_3, x_4$  so  $\bar{x}$  has min length:  $x_3 = 0$   
 $x_4 = 0$

$$\text{Then } x^+ = \begin{bmatrix} b_1 \\ \frac{b_1}{\sigma_1} \\ b_2 \\ \frac{b_2}{\sigma_2} \\ 0 \\ 0 \end{bmatrix}$$

and what is  $A^+$  such that  $A^+ b = x^+ ?$

By inspection  $A^+ = \begin{bmatrix} \frac{1}{\sigma_1} & 0 & 0 \\ 0 & \frac{1}{\sigma_2} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$  we had to transpose non-zero diag elts, and transpose matrix.

Lemma The least sq soln to  $\sum x = b$  is  $x^+ = \Sigma^+ b$

Pf  $x^+ = \Sigma^+ b = \begin{bmatrix} (\Delta^r)^r & O_r^e \\ O_k^r & O_k^e \end{bmatrix} \begin{bmatrix} b_r^r \\ b_e^e \end{bmatrix} = \begin{bmatrix} \Delta^r b_r^r \\ O_k^r b_e^e \end{bmatrix}$  co-ords for basis vectors  $x_1, \dots, x_r$   $\Rightarrow$  row space

$\begin{bmatrix} r+l=m \\ r+k=n \text{ as before} \end{bmatrix}$

Thus we see  $x^+$  in row space

Now we want to show  $p_b = \Sigma \Sigma^+ b$  and it will be of interest to do it by multiplying  $\Sigma \Sigma^+$  first:

$$\sum_m \begin{bmatrix} \Delta_r^r & O_r^k \\ O_e^r & O_e^k \end{bmatrix} \begin{bmatrix} (\Delta^r)^r & O_r^e \\ O_k^r & O_k^e \end{bmatrix} \begin{bmatrix} b_r^r \\ b_e^e \end{bmatrix} = \begin{bmatrix} \Delta_r^r (\Delta^r)^r + O_r^k O_r^r & \Delta_r^r O_r^e + O_r^k O_e^r \\ O_e^r (\Delta^r)^r + O_e^k O_r^r & O_e^r O_r^e + O_e^k O_e^r \end{bmatrix} \begin{bmatrix} b_r^r \\ b_e^e \end{bmatrix}$$

$$m \left\{ \begin{bmatrix} I_r^r & O_r^e \\ O_e^r & O_e^e \end{bmatrix} \begin{bmatrix} b_r^r \\ b_e^e \end{bmatrix} \right\} = \begin{bmatrix} b_r^r \\ b_e^e \end{bmatrix} = p_b \quad \checkmark$$

□

Now we need to prove the thm →

Repeat Thm: The min length least sq soln to  $Ax=b$  is  $x^+ = A^+b$

Pf. Want to minimize  $\|Ax-b\| = \|Q_1 \Sigma Q_2^T x - b\|$

$$= \|Q_1^T(Q_1 \Sigma Q_2^T x - b)\| \quad \begin{matrix} \text{we can mult by ON matrix} \\ \text{w/out changing length} \end{matrix}$$

$$= \|\sum(Q_2^T x) - Q_1^T b\| \quad y := Q_2^T x$$

$$= \|\sum y - Q_1^T b\|$$

So we want min length soln to  $\sum y = Q_1^T b$  and from the Lemma  
we know this is  $y^+ = \sum^+(Q_1^T b)$

Transform back to  $x$ :  $x^+ = Q_2 y^+ = (Q_2 \sum^+ Q_1^T) b = A^+ b$   $\square$

Strong asks us to validate:

- $x^+$  is in the row space of  $A$   $[\exists z \in A^T z = x^+]$
- $Ax^+ = P_b$

For  $Ax^+ = P_b$ , we are showing  $AA^+b = Q_1 \sum Q_2^T (Q_2 \sum^+ Q_1^T) b$

$$= Q_1 \sum \sum^+ Q_1^T b$$

$$= Q_1 \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} Q_1^T b \quad \text{from prev lemma}$$

$$= \begin{bmatrix} 1 & 0 & \dots & 0 \\ b_1 & b_2 & \dots & b_m \\ 0 & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} -b_1 \\ -b_2 \\ \vdots \\ -b_m \end{bmatrix} [b]$$

Really it is

$$Q_1 \begin{bmatrix} -b_1 \\ -b_2 \\ \vdots \\ -b_m \\ 0 \end{bmatrix} [b] = Q_1 \begin{bmatrix} b^T b \\ b_1^T b \\ b_2^T b \\ \vdots \\ b_m^T b \\ 0 \end{bmatrix} \leftarrow \begin{matrix} \text{This vector is the proj of original } b \\ \text{into Col}(A) [\text{i.e. } P_b] \end{matrix}$$

and  $Q_1$  is COB to put it in terms of orig basis for  $\mathbb{R}^m$ .