

# SINGULAR VALUE DECOMPOSITION

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Wednesday, November 3, 2021

# LOGISTICS

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## General announcements

- Let me know if you have concerns about your grades (disagreements, etc.)
- Be careful with honor code

## Office hours on Friday November 05, 2021

- 8am-9:30am on BlueJeans ([BlueJeans](#))
- Focus on Midterm 2 preparation

## Midterm 2:

- Moved to **Monday November 8, 2021** (gives you weekend to prepare)
- Coverage: everything since Midterm 1 (dont' forget the fundamentals though), emphasis on **regression**

# WHAT'S ON THE AGENDA FOR TODAY?

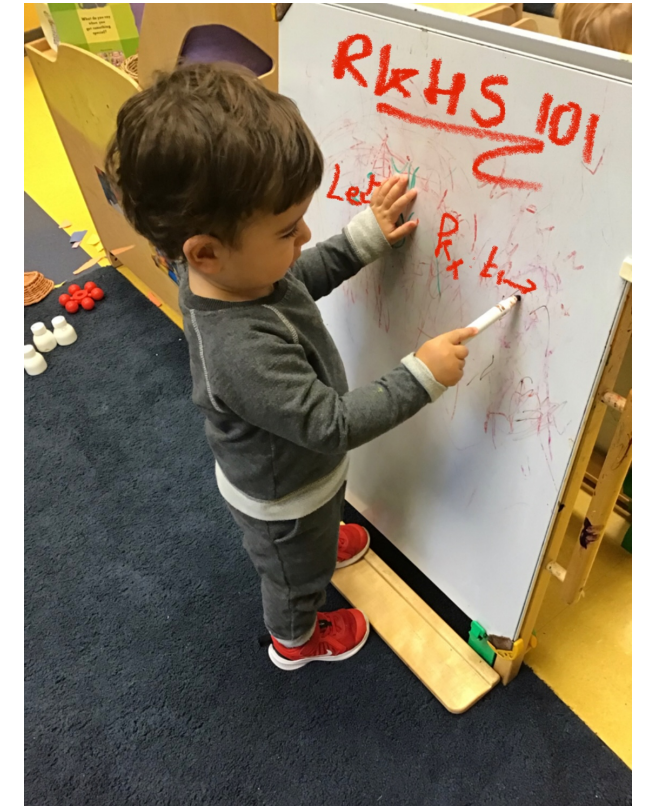
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Last time:

- Symmetric matrices and spectral theorem
- *Objective*: further understand least-square problems

Today: singular value decomposition

Reading: lecture notes 12/13



Toddlers can do it!

# SPECTRAL THEOREM

## Lemma (Existence of eigenvector)

Every complex matrix  $\mathbf{A}$  has at least one complex eigenvector and every real symmetric matrix has real eigenvalues and at least one real eigenvector.

**Lemma (Schur triangularization lemma)** Every matrix  $\mathbf{A} \in \mathbb{C}^{n \times n}$  is unitarily similar to an upper triangular matrix, i.e.,

$$\mathbf{A} = \mathbf{V} \mathbf{\Delta} \mathbf{V}^\dagger$$

with  $\mathbf{\Delta}$  upper triangular and  $\mathbf{V}^\dagger = \mathbf{V}^{-1}$ .

**Theorem (Spectral theorem)** Every hermitian matrix is unitarily similar to a real-valued diagonal matrix.

Note that if  $\mathbf{A} = \mathbf{V} \mathbf{D} \mathbf{V}^\dagger$  then

$$\mathbf{A} = \sum_{i=1}^n \lambda_i \underbrace{\mathbf{v}_i \mathbf{v}_i^\dagger}_{\text{rank } 1}$$

How about real-valued matrices  $\mathbf{A} \in \mathbb{R}^{n \times n}$ ?

Every symmetric matrix can be diagonalized in an orthonormal basis of eigenvectors ( $A = V D V^T$  w/  $V^T V = V V^T = I$ )

# SYMMETRIC POSITIVE DEFINITE MATRICES

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## Definition.

A symmetric matrix  $\mathbf{A}$  is positive definite if it has positive eigenvalues, i.e.,  $\forall i \in \{1, \dots, n\} \lambda_i > 0$ .

A symmetric matrix  $\mathbf{A}$  is positive semidefinite if it has nonnegative eigenvalues, i.e.,  $\forall i \in \{1, \dots, n\} \lambda_i \geq 0$ .

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Convention:  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$

Variational form of extreme eigenvalues for symmetric positive definite matrices  $\mathbf{A}$

$$\lambda_1 = \max_{\mathbf{x} \in \mathbb{R}^n: \|\mathbf{x}\|_2=1} \mathbf{x}^\top \mathbf{A} \mathbf{x} = \max_{\mathbf{x} \in \mathbb{R}^n} \frac{\mathbf{x}^\top \mathbf{A} \mathbf{x}}{\|\mathbf{x}\|_2^2}$$
$$\lambda_n = \min_{\mathbf{x} \in \mathbb{R}^n: \|\mathbf{x}\|_2=1} \mathbf{x}^\top \mathbf{A} \mathbf{x} = \min_{\mathbf{x} \in \mathbb{R}^n} \frac{\mathbf{x}^\top \mathbf{A} \mathbf{x}}{\|\mathbf{x}\|_2^2}$$

Note:

$$\max_{x \in \mathbb{R}^n} \frac{x^T A x}{\|x\|_2^2} = \max_{x \in \mathbb{R}^n} \underbrace{\left(\frac{x}{\|x\|_2}\right)^T}_{\triangleq v \text{ and } \|v\|_2 = 1} A \underbrace{\left(\frac{x}{\|x\|_2}\right)}_{\|x\|_2 = 1} = \max_{\substack{x \in \mathbb{R}^n \\ \|x\|_2 = 1}} x^T A x$$

Recall that  $A = V D V^T$  so that we look for  $\max_{x \in \mathbb{R}^n: \|x\|_2 = 1} x^T V D V^T x$  wr  $\|u\|_2^2 = u^T u = x^T V V^T x = x^T x$

$$\text{i.e. } \max_{u \in \mathbb{R}^n: \|u\|_2 = 1} u^T D u = \max_{u \in \mathbb{R}^n: \|u\|_2 = 1} \sum_{i=1}^n \lambda_i u_i^2 \quad (*)$$

$$(*) \quad \sum_{i=1}^n \lambda_i u_i^2 \leq \lambda_1 \sum_{i=1}^n u_i^2 = \lambda_1 \quad \text{achieved wr } \underline{u} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (\text{assuming } D = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix})$$

$$u = V^T x \quad \text{so that } x = V u = \begin{pmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_n \\ | & | & & | \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = v_1$$

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$$\lambda_n = \min_{\mathbf{x} \in \mathbb{R}^n: \|\mathbf{x}\|_2=1} \mathbf{x}^\top \mathbf{A} \mathbf{x} = \min_{\mathbf{x} \in \mathbb{R}^n} \frac{\mathbf{x}^\top \mathbf{A} \mathbf{x}}{\|\mathbf{x}\|_2^2}$$

## Theorem (Sylvester theorem)

For any analytic function  $f$ , we have

$$f(\mathbf{A}) = \sum_{i=1}^n f(\lambda_i) \mathbf{v}_i \mathbf{v}_i^\top$$



"Proof": Let  $A$  be symmetric matrix so that  $A = \sum_{i=1}^n \lambda_i v_i v_i^T$  ( $A \in \mathbb{R}^{n \times n}$ )  $\{v_i\}_{i=1}^n$  orthonormal basis of eigenvectors

$$\text{Then } A^2 = A \times A = \left( \sum_{i=1}^n \lambda_i v_i v_i^T \right) \left( \sum_{j=1}^n \lambda_j v_j v_j^T \right) = \sum_{i=1}^n \sum_{j=1}^n \lambda_i \lambda_j \underbrace{v_i v_i^T v_j v_j^T}_{\langle v_i, v_j \rangle = \delta_{ij} \triangleq \begin{cases} 1 & \text{if } i=j \\ 0 & \text{else} \end{cases}} = \sum_{i=1}^n \lambda_i^2 v_i v_i^T$$

By extension  $A^p = \sum_{i=1}^n \lambda_i^p v_i v_i^T$

$$\text{poly}(A) = \sum_{i=1}^n \text{poly}(\lambda_i) v_i v_i^T$$

Finally for any  $f$  analytic  $f(A) = \sum_{i=1}^n f(\lambda_i) v_i v_i^T$

Example:  $A^{-1} = \sum_{i=1}^n \frac{1}{\lambda_i} v_i v_i^T$  (Assuming  $\forall_i \lambda_i \neq 0$ )



Note, assume  $v_1$  eigenvector associated to  $\lambda_1$  wlog  $\|v_1\| = \|v_2\| = 1$   
-----  $v_2$  ----- to  $\lambda_2 \neq \lambda_1$

$$\begin{aligned} \text{Note that } v_2^T A v_1 &= v_2^T (A v_1) = \lambda_1 v_2^T v_1 \\ &= (v_2^T A) v_1 = (v_2^T A^T) v_1 = (A v_2)^T v_1 = \lambda_2 v_2^T v_1 \end{aligned}$$

$$\text{Hence } \underbrace{(\lambda_1 - \lambda_2)}_{\neq 0} v_2^T v_1 = 0 \quad \text{hence } v_2^T v_1 = 0$$

In addition:  $A^{1/2} = \sum_{i=1}^n \sqrt{\lambda_i} v_i v_i^T = V \Lambda^{1/2} V^T$

$\uparrow$   
A SPD

$$\exp(A) = \sum_{i=1}^n e^{\lambda_i} v_i v_i^T$$

# SYSTEM OF SYMMETRIC DEFINITE EQUATIONS

Consider the system  $\mathbf{y} = \mathbf{A}\mathbf{x}$  with  $\mathbf{A}$  symmetric positive definite

**Proposition.**

Let  $\{\mathbf{v}_i\}$  be the eigenvectors of  $\mathbf{A}$ .

$$\mathbf{x} = \sum_{i=1}^n \frac{1}{\lambda_i} \langle \mathbf{y}, \mathbf{v}_i \rangle \mathbf{v}_i$$

Assume some observation error  $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{e}$ , with  $\mathbf{e}$  unknown, and we reconstruct  $\mathbf{x}$  as  $\tilde{\mathbf{x}}$  by applying  $\mathbf{A}^{-1}$

**Proposition (Worst case bounds)**

$$\frac{1}{\lambda_1^2} \|\mathbf{e}\|_2^2 \leq \|\mathbf{x} - \tilde{\mathbf{x}}\|_2 \leq \frac{1}{\lambda_n^2} \|\mathbf{e}\|_2^2.$$

**Proposition (Average case bound)** If  $\mathbf{e} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ , then

$$\mathbb{E} [\|\mathbf{x} - \tilde{\mathbf{x}}\|_2] = \sigma^2 \sum_{i=1}^n \frac{1}{\lambda_i^2}$$

Proof:  $A$  symmetric definite in  $\mathbb{R}^{n \times n}$

In that case  $y = Ax$  has a unique solution  $x = A^{-1}y = \left( \sum_{i=1}^n \frac{1}{d_i} v_i v_i^T \right) y = \sum_{i=1}^n \frac{1}{d_i} v_i (v_i^T y)$

$$= \sum_{i=1}^n \frac{1}{d_i} \langle v_i, y \rangle v_i$$



Proof:  $y = Ax + e$  ( $A$  symmetric definite)

$$\tilde{x} \triangleq A^{-1}y = A^{-1}(Ax + e) = x + A^{-1}e \quad (*) \quad \text{note that } A^{-1} = \sum_{i=1}^n \frac{1}{d_i} v_i v_i^T$$

The reconstruction error is  $x - \tilde{x}$

$$\begin{aligned} \|x - \tilde{x}\|_2^2 &= \|A^{-1}e\|_2^2 = e^T A^{-1T} A^{-1} e = e^T \left( \sum_{i=1}^n \frac{1}{d_i} v_i v_i^T \right) \left( \sum_{j=1}^n \frac{1}{d_j} v_j v_j^T \right) e = e^T \sum_{i=1}^n \frac{1}{d_i^2} v_i v_i^T e \\ &= \sum_{i=1}^n \frac{1}{d_i^2} \underbrace{e^T v_i v_i^T e}_{\triangleq \langle e, v_i \rangle^2} \end{aligned}$$

Hence  $\|x - \tilde{x}\|_2^2 \leq \frac{1}{d_n^2} \sum_{i=1}^n \langle e, v_i \rangle^2 = \frac{1}{d_n^2} \|e\|_2^2$

Similarly  $\|x - \tilde{x}\|_2^2 \geq \frac{1}{d_{\max}^2} \|e\|_2^2$

influence of noise itself

effect of  $A^{-1}$

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**Proposition (Average case bound)** If  $\mathbf{e} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$ , then

$$\mathbb{E} [\|\mathbf{x} - \tilde{\mathbf{x}}\|_2] = \sigma^2 \sum_{i=1}^n \frac{1}{\lambda_i^2} = \overbrace{n\sigma^2}^{\mathbb{E}(\|\mathbf{e}\|_2^2)} \underbrace{\frac{1}{n} \sum_{i=1}^n \frac{1}{\lambda_i^2}}_{\text{average of } \frac{1}{\lambda_i^2}}$$

# SINGULAR VALUE DECOMPOSITION

What happens for non-square matrices?

## Theorem (Singular value decomposition)

Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with  $\text{rank}(\mathbf{A}) = r$ . Then  $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$  where

- $\mathbf{U} \in \mathbb{R}^{m \times r}$  such that  $\mathbf{U}^T\mathbf{U} = \mathbf{I}_r$  (orthonormal columns) (in general  $\mathbf{U}\mathbf{U}^T \neq \mathbf{I}$ )
- $\mathbf{V} \in \mathbb{R}^{n \times r}$  such that  $\mathbf{V}^T\mathbf{V} = \mathbf{I}_r$  (orthonormal columns) (in general  $\mathbf{V}\mathbf{V}^T \neq \mathbf{I}$ )
- $\mathbf{\Sigma} \in \mathbb{R}^{r \times r}$  is diagonal with *positive entries*

$$\mathbf{\Sigma} \triangleq \begin{bmatrix} \sigma_1 & 0 & 0 & \cdots \\ 0 & \sigma_2 & 0 & \cdots \\ \vdots & & \ddots & \\ 0 & \cdots & \cdots & \sigma_r \end{bmatrix}$$

and  $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ . The  $\sigma_i$  are called the *singular values*

We say that  $\mathbf{A}$  is full rank if  $r = \min(m, n)$

We can write  $\mathbf{A} = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T$

Proof:  $A \in \mathbb{R}^{m \times n}$ ; form  $A^T A \in \mathbb{R}^{n \times n}$ , is symmetric and can be written  $A^T A = \sum_{i=1}^n d_i v_i v_i^T$

Note  $\forall x \in \mathbb{R}^n$   $x^T A^T A x = \|Ax\|_2^2 \geq 0$  so that  $\forall i \in \llbracket 1, n \rrbracket$   $d_i \geq 0$

Assume  $\text{rank}(A) = r$  then  $\text{rank}(A^T A) = r$  (prove it!) so that  $d_1 \geq d_2 \geq \dots \geq d_r > 0$   $d_{r+1} \dots d_n = 0$

For  $i \in \llbracket 1, r \rrbracket$  set  $u_i \stackrel{\Delta}{=} \frac{1}{\sqrt{d_i}} A v_i$

① Check  $\{u_i\}_{i=1}^r$  are orthonormal

$$\forall 1 \leq i \leq j \leq r \quad u_i^T u_j = \frac{1}{\sqrt{d_i d_j}} v_j^T A^T A v_i = \frac{1}{\sqrt{d_i d_j}} v_j^T \left( \sum_{\ell=1}^n d_\ell v_\ell v_\ell^T \right) v_i = \begin{cases} 1 & \text{if } j=i \\ 0 & \text{else} \end{cases}$$