Mathematics Methods for Computer Science

Motivation

SVD

Pseudoinverses

ow-Rank Approx.

Matrix Norms

Damilania etian

PCA

## Mathematics Methods for Computer Science

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Mathematics Methods for Computer Science

Motivation

**SVD** 

Pseudoinverse:

Low-Rank Approx

Matrix Norme

Procrustes Problem

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## Lecture

Singular Value Decomposition

## Understanding the Geometry of $A \in \mathbb{R}^{m \times n}$

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## Critical points of the ratio:

$$R(\vec{v}) = \frac{||A\vec{v}||_2}{||\vec{v}||_2}$$

## Understanding the Geometry of $A \in \mathbb{R}^{m \times n}$

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## Critical points of the ratio:

$$R(\vec{v}) = \frac{||A\vec{v}||_2}{||\vec{v}||_2}$$

• 
$$R(\alpha \vec{v}) = R(\vec{v}) \Rightarrow \mathsf{take} \ ||\vec{v}||_2 = 1$$

• 
$$R(\vec{v}) \geq 0 \Rightarrow$$
 study  $R^2(\vec{v})$  instead

## Once Again...

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Critical points satisfy  $A^{\top}A\vec{v}_i = \lambda_i \vec{v}_i$ .

## Once Again...

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## Critical points satisfy $A^{\top}A\vec{v}_i = \lambda_i \vec{v}_i$ .

## **Properties:**

- $\lambda_i \geq 0 \ \forall i$
- Basis is full and orthonormal

## Geometric Question

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# What about A instead of $A^{\top}A$ ?

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What about A instead of  $A^{\top}A$ ?

Object of study:  $\vec{u}_i \equiv A\hat{v}_i$ 

## Observation

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#### Lemma

Either  $\vec{u}_i = \vec{0}$  or  $\vec{u}_i$  is an eigenvector of  $AA^{\top}$  with

$$||\vec{u}_i||_2 = \sqrt{\lambda_i}||\hat{v}_i||_2 = \sqrt{\lambda_i}.$$

### Lemma

## Simpler proof than in book (top p. 132):

$$A^{\top}A\hat{v}_i = \lambda_i\hat{v}_i$$
 $AA^{\top}(A\hat{v}_i) = \lambda_iA\hat{v}_i$ 
 $AA^{\top}\vec{v}_i = \lambda_i\vec{v}_i$ 

Length of  $\vec{u}_i = A\hat{v}_i$  follows from

$$\|\vec{u}_i\|_2^2 = \|A\hat{v}_i\|_2^2 = \hat{v}_i^{\top} A^{\top} A \hat{v}_i = \lambda_i \hat{v}_i^{\top} \hat{v}_i = \lambda_i$$

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## Corresponding Eigenvalues

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$$k = \text{ number of } \lambda_i > 0$$
 
$$A^\top A \hat{v}_i = \lambda_i \hat{v}_i$$
 
$$AA^\top \hat{u}_i = \lambda_i \hat{u}_i$$
 
$$\bar{U} \in \mathbb{R}^{n \times k} = \text{ matrix of unit } \hat{u}_i \text{ 's }$$
 
$$\bar{V} \in \mathbb{R}^{m \times k} = \text{ matrix of unit } \hat{v}_i \text{ 's }$$

### Observation

Simpler lemma + proof than book (bottom p.132):

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## Lemma

$$\hat{u}_i^{\top} A \hat{v}_j = \sqrt{\lambda_i} \delta_{ij}$$

$$\bar{\Sigma} \equiv diag(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_k})$$

$$= diag(\sigma_i, \cdots, \sigma_k)(\sigma_i \text{ are singular values})$$

## Observation

Simpler lemma + proof than book (bottom p.132):

## Lemma

$$\hat{u}_i^{\top} A \hat{v}_j = \sqrt{\lambda_i} \delta_{ij}$$

$$\bar{\Sigma} \equiv diag(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_k})$$

$$= diag(\sigma_i, \cdots, \sigma_k)(\sigma_i \text{ are singular values})$$

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## Corollary

$$\bar{U}^{\top}A\bar{V} = \bar{\Sigma}$$

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## Fat SVD: Completing the Basis

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Add 
$$\hat{v}_i$$
 with  $A^{\top}A\vec{\hat{v}}_i=\vec{0}$  and  $\hat{u}_i$  with  $AA^{\top}\hat{u}_i=\vec{0}$ 

## Fat SVD: Completing the Basis

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## Add $\hat{v}_i$ with $A^{\top}A\vec{\hat{v}}_i=\vec{0}$ and $\hat{u}_i$ with $AA^{\top}\hat{u}_i=\vec{0}$

$$\bar{U} \in \mathbb{R}^{m \times k}, \bar{V} \in \mathbb{R}^{n \times k} \mapsto U \in \mathbb{R}^{m \times m}, V \in \mathbb{R}^{n \times n}$$

## Fat SVD: Completing the Basis

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Add 
$$\hat{v}_i$$
 with  $A^{\top}A\vec{\hat{v}_i}=\vec{0}$  and  $\hat{u}_i$  with  $AA^{\top}\hat{u}_i=\vec{0}$ 

$$ar{U} \in \mathbb{R}^{m imes k}, ar{V} \in \mathbb{R}^{n imes k} \mapsto \ U \in \mathbb{R}^{m imes m}, V \in \mathbb{R}^{n imes n}$$

$$\Sigma_{ij} \equiv \left\{ \begin{array}{c} \sqrt{\lambda_i} \ i = j \ \text{and} \ i \leq k \\ 0 \end{array} \right. \quad \text{otherwise}$$

## Singular Value Decomposition

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$$A = U\Sigma V^{\top}$$

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## Geometry of Linear Transformations

 $A = U\Sigma V^{\top}$ 

- Rotate  $(V^{\top})$ 
  - Scale  $(\Sigma)$
  - Rotate (U)

Motivation

SVD

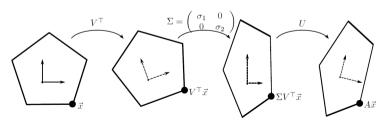
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## SVD Vocabulary

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$$A = U\Sigma V^{\top}$$

• Left singular vectors:

Columns of U; span col A

Right singular vectors:

Columns of V; span row A

• Singular values:

Diagonal  $\sigma_i$  of  $\Sigma$ ; sort  $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$ 

## Computing SVD: Simple Strategy

ullet Columns of V are eigenvectors of  $A^{\top}A$ 

•  $AV = U\Sigma \Rightarrow$  columns of U corresponding to nonzero singular values are normalized columns of AV

• Remaining columns of U satisfy  $AA^{\top}\vec{u}_i = \vec{0}$ .

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**SVD** 

## Computing SVD: Simple Strategy

• Columns of V are eigenvectors of  $A^{\top}A$ 

•  $AV = U\Sigma \Rightarrow$  columns of U corresponding to nonzero singular values are normalized columns of AV

• Remaining columns of U satisfy  $AA^{\top}\vec{u}_i = \vec{0}$ .  $\exists$  more specialized methods!

## Solving Linear Systems with $A = U\Sigma V^{\top}$

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$$A\vec{x} = \vec{b}$$

$$\Longrightarrow U\Sigma V^{\top}\vec{x} = \vec{b}$$

$$\Longrightarrow \vec{x} = V\Sigma^{-1}U^{\top}\vec{b}$$

## Solving Linear Systems with $A = U\Sigma V^{\top}$

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$$A\vec{x} = \vec{b}$$
  $\Longrightarrow U\Sigma V^{\top}\vec{x} = \vec{b}$   $\Longrightarrow \vec{x} = V\Sigma^{-1}U^{\top}\vec{b}$  What is  $\Sigma^{-1}$ ?

## Uniting Short/Tall Matrices

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DC A

## Simplification

Motivation

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#### Pseudoinverses

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Matrix Norm

Matrix Morms

Regularization

Procrustes Problem

$$A^{\top}A = V \Sigma^{\top} \Sigma V^{\top}$$

## Simplification

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$$A^{\top}A = V \Sigma^{\top} \Sigma V^{\top}$$

$$A^{\top}A\vec{x} = A^{\top}\vec{b} \Leftrightarrow \Sigma^{\top}\Sigma\vec{y} = \Sigma^{\top}\vec{d}$$
$$\vec{y} \equiv V^{\top}\vec{x}$$
$$\vec{d} \equiv U^{\top}\vec{b}$$

## Resulting Optimization

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minimize 
$$||\vec{y}||_2^2$$
 such that  $\Sigma^{\top}\Sigma\vec{y}=\Sigma^{\top}\vec{d}$ 

## Solution

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$$\Sigma_{ij}^{+} \equiv \begin{cases} 1/\sigma_{i} & i = j, \sigma_{i} \neq 0, \text{ and } i \leq k \\ 0 & \text{otherwise} \end{cases}$$

$$\implies \vec{y} = \Sigma^{+} \vec{d}$$

$$\implies \vec{x} = V \Sigma^{+} U^{\top} \vec{b}$$

## Pseudoinverse

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#### **Pseudoinverses**

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$$A^+ = V \Sigma^+ U^\top$$

## Pseudoinverse Properties

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• A square and invertible  $\Rightarrow A^+ = A^{-1}$ 

ullet A **overdetermined**  $\Rightarrow$  A $^+ ec{b}$  gives least-squares

• A **underdetermined**  $\Rightarrow$  A<sup>+</sup> $\vec{b}$  gives least-squares solution to  $A\vec{x} \approx \vec{b}$  with least (Euclidean) norm

## Alternative Form

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$$A = U\Sigma V^{\top} \Longrightarrow A = \sum_{i=1}^{\ell} \sigma_i \vec{u}_i \vec{v}_i^{\top}$$
$$\ell \equiv \min\{m, n\}$$

## Outer Product

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$$\vec{u} \otimes \vec{v} \equiv \vec{u} \vec{v}^{\top}$$

## Computing $A\vec{x}$

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$$A\vec{x} = \sum_{i} \sigma_i (\vec{v}_i \cdot \vec{x}) \vec{u}_i$$

## Computing $A\vec{x}$

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$$A\vec{x} = \sum_{i} \sigma_i (\vec{v}_i \cdot \vec{x}) \vec{u}_i$$

# Trick: Ignore small $\sigma_i$ .

## Computing $A^+\vec{x}$

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$$A^{+} = \sum_{\sigma_i \neq 0} \frac{\vec{v}_i \vec{u}_i^{\top}}{\sigma_i}$$

# Trick: Ignore large $\sigma_i$ .

## Even Better Trick

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# Do not compute large (small) $\sigma_i$ at all!

## Eckart-Young Theorem

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#### Theorem

Suppose  $\tilde{A}$  is obtained from  $A=U\Sigma V^{\top}$  by truncating all but the k largest singular values  $\sigma_i$  of A to zero. Then,  $\tilde{A}$  minimizes both  $||A-\tilde{A}||_{Fro}$  and  $||A-\tilde{A}||_2$  subject to the constraint that the column space of  $\tilde{A}$  has at most dimension k.

## Matrix Norm Expressions

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$$||A||_{Fro}^2 = \sum \sigma_i^2$$

$$||A||_2 = max\{\sigma_i\}$$

$$cond\ A = \sigma_{max}/\sigma_{min}$$

## Revisiting Tikhonov Regularization

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Regularized least-squares problem:

$$(A^{\top}A + \alpha I)\vec{x} = A^{\top}\vec{b}.$$

Perform SVD analysis.

What does  $\alpha$  do to the singular values?

Example: Vandermonde matrix, V

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## Rigid Alignment

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Point cloud 1



Point cloud 2



Initial alignment



Final alignment

#### Variational Formulation

Given  $\vec{x}_{1i} \mapsto \vec{x}_{2i}$ 

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$$\min_{R^{\top}R = I_{3\times 3}, \vec{t} \in \mathbb{R}^3} \sum_{i} ||R\vec{x}_{1i} + \vec{t} - \vec{x}_{2i}||_2^2$$

## Variational Formulation

Given 
$$\vec{x}_{1i} \mapsto \vec{x}_{2i}$$

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$$\min_{R^{\top}R = I_{3\times 3}, \vec{t} \in \mathbb{R}^3} \sum_{i} ||R\vec{x}_{1i} + \vec{t} - \vec{x}_{2i}||_2^2$$

#### Alternate:

- Minimize with respect to  $\vec{t}$ : Least-squares
- Minimize with respect to R: SVD



## Procrustes via SVD

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$$\min_{R^{\top}R = I_{3 \times 3}} ||RX_1 - X_2^t||_{Fro}^2$$

#### Procrustes via SVD

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$$\min_{R^{\top}R = I_{3\times 3}} ||RX_1 - X_2^t||_{Fro}^2$$

## Orthogonal Procrustes Theorem

The orthogonal matrix R minimizing  $||RX-Y||^2$  is given by  $UV^{\top}$ , where SVD is applied to factor  $YX^{\top} = U\Sigma V^{\top}$ .

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# Application: As-Rigid-As-Possible

# As-Rigid-As-Possible Surface Modeling

Olga Sorkine and Marc Alexa Eurographics/ACM SIGGRAPH Symposium on Geometry Processing 2007.

http://www.youtube.com/watch?v=ltX-qUjbkdc



## Related: Polar Decomposition

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# F = Ru Special case:

- F is square real-valued matrix;
- R is best rotation matrix approximation;
- ullet U is right symmetric PSD stretch matrix.
- Proof by SVD.

#### Recall: Statistics Problem

**Given:** Collection of data points  $\vec{x}_i$ 

- Age
- Weight
- Blood pressure
- Heart rate

Find: Correlations between different dimensions

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## Simplest Model

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# One-dimensional subspace

$$\vec{x}_i \approx c_i \vec{v}$$

#### More General Statement

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#### Principal Component Analysis

The matrix  $C \in \mathbb{R}^{n \times d}$  minimizing  $||X - CC^{\top}X||_{Fro}$  subject to  $C^{\top}C = I_{d \times d}$  is given

by the first d columns of U, for  $X = U\Sigma V^{\top}$ .

Proved in textbook.

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# Application: Eigenfaces

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(a) Input faces

(b) Eigenfaces



$$=-13.1\times$$





(c) Projection

 $+ \cdots$