Mathematics Methods for Computer Science

Motivation

SVD

Pseudoinverses

Low-Rank Approx.

Matrix Norms

Wath North

Regularization

Procrustes Problem

PCA

Mathematics Methods for Computer Science

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SJTU-SE DALAB



Mathematics Methods for Computer Science

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Lecture

Singular Value Decomposition

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

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Critical points of the ratio:

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

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Procrustes Problem

PC/

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...

Motivation

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Procrustes Problen

$$R^2(\vec{v}) = \|A\vec{v}\|_2^2 = \vec{v}A^{\top}A\vec{v}$$

Critical points of
$$\vec{v}A^{\top}A\vec{v}$$
 s.t. $\|\vec{v}\|_2 = 1$ $\Rightarrow \vec{v}_i$ satisfying $A^{\top}A\vec{v}_i = \lambda_i \vec{v}_i$

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$$R^2(\vec{v}) = \|A\vec{v}\|_2^2 = \vec{v}A^{\top}A\vec{v}$$

Critical points of
$$\vec{v}A^{\top}A\vec{v}$$
 s.t. $\|\vec{v}\|_2 = 1$ $\Rightarrow \vec{v}_i$ satisfying $A^{\top}A\vec{v}_i = \lambda_i\vec{v}_i$

Properties: $A^{T}A$ is symmetric positive semidefinite

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

Geometric Question

Motivation

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

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Matrix Norms

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PCA

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

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

Observation

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Pseudoinverse:

Low-Rank Approx

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Matrix Morni

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Lemma

Either $\vec{u}_i = \vec{0}$ or \vec{u}_i is an eigenvector of AA^{\top} with $\|\vec{u}_i\|_2 = \sqrt{\lambda_i} \|\hat{v}_i\|_2 = \sqrt{\lambda_i}$.

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

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

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

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

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

Motivation

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

Lemma

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

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

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

Observation

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

Lemma

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

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

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

Corollary

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

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Matrix Norm

Daniel de la contraction

Procrustes Problen

PC/

Fat SVD: Completing the Basis

Motivation

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

Motivation

Motivatio

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Matrix Norms

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

Motivation

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Procrustes Problem

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

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

$$\Sigma_{ij} \equiv \begin{cases} \sqrt{\lambda_i}, & i = j \text{ and } i \leq k \\ 0, & \text{otherwise} \end{cases}$$

Singular Value Decomposition

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SVD

Pseudoinverses

Low-Rank Approx

Matrix Norms

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D . D ...

DC A

$$A=U\Sigma V$$
 $^{ op}$ U/V为正交矩阵 ,是对角矩阵

Geometry of Linear Transformations

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

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

Motivation

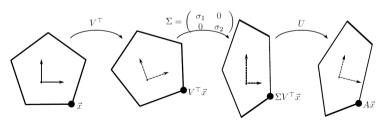
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Matrix Norms

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PCA

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

• Left singular vectors:

Columns of U; span col A

• Right singular vectors:

Columns of V; span row A

Singular values:

Diagonal σ_i of Σ ; sort $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$

Computing SVD: Simple Strategy

Motivatio

SVD

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Procruetes Problem

PCA

• 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 $AA^{\top}\vec{u}_i = \vec{0}$.

Computing SVD: Simple Strategy

Motivation

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Low-Rank Approx

Matrix Norma

Draguetas Drahlan

PC*A*

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

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

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

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

Motivation

Pseudoinverses

Low-Marik Approx.

Matrix Norms

Regularization

Procrustes Problem

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

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

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

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

Motivation

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Pseudoinverses

Low-Rank Approx

Matrix Norms

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D . D ...

DC A

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

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

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

What is Σ^{-1} ?

为 中对角线上元素全部取倒数得到的矩阵

Uniting Short/Tall Matrices

Motivation

SVD

Pseudoinverses

Low-Rank Approx.

Matrix Norms

Regularization

Procrustes Problem

Simplification

Pseudoinverses

$$\begin{split} \boldsymbol{A}^{\top} \boldsymbol{A} &= \left(\boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top}\right)^{\top} \left(\boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top}\right) \\ &= \boldsymbol{V} \boldsymbol{\Sigma}^{\top} \boldsymbol{U}^{\top} \boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top} \text{ since } (\boldsymbol{A} \boldsymbol{B})^{\top} = \boldsymbol{B}^{\top} \boldsymbol{A}^{\top} \\ &= \boldsymbol{V} \boldsymbol{\Sigma}^{\top} \boldsymbol{\Sigma} \boldsymbol{V}^{\top} \text{ since } \boldsymbol{U} \text{ is orthogonal.} \end{split}$$

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

Simplification

Pseudoinverses

$$\begin{split} \boldsymbol{A}^{\top} \boldsymbol{A} &= \left(\boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top}\right)^{\top} \left(\boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top}\right) \\ &= \boldsymbol{V} \boldsymbol{\Sigma}^{\top} \boldsymbol{U}^{\top} \boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top} \text{ since } (\boldsymbol{A} \boldsymbol{B})^{\top} = \boldsymbol{B}^{\top} \boldsymbol{A}^{\top} \\ &= \boldsymbol{V} \boldsymbol{\Sigma}^{\top} \boldsymbol{\Sigma} \boldsymbol{V}^{\top} \text{ since } \boldsymbol{U} \text{ is orthogonal.} \end{split}$$

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

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

Resulting Optimization

Motivation

3 V D

Pseudoinverses

Low-Rank Approx

Matrix Norm

Regularization

Procrustes Problen

Resulting Optimization

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PCA

$$\begin{array}{c} \text{minimize } ||\vec{y}||_2^2 \\ \text{such that } \Sigma^\top \Sigma \vec{y} = \Sigma^\top \vec{d} \end{array}$$

因为对角阵与其转置的乘积就是原对角矩阵对角线上的元素平方得到的矩阵

$$\Sigma^{\top}\Sigma\vec{y} = \Sigma^{\top}\vec{d} \implies \sigma_i^2 y_i = \sigma_i d_i$$

$$y_i = \left\{ egin{array}{ll} rac{d_i}{\sigma_i} & \sigma_i
eq 0 \\ ext{no constraint (take 0)} & \sigma_i = 0 \end{array}
ight.$$

Solution

Motivation

SVD

Pseudoinverses

Low-Rank Approx

Matrix Norms

....

DC A

$$\Sigma_{ij}^{+} \equiv \left\{ \begin{array}{ll} 1/\sigma_{i} & i=j, \sigma_{i} \neq 0 \\ 0 & \text{otherwise} \end{array} \right.$$

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

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

Pseudoinverse

矩阵A^+称为矩阵A的伪逆矩阵

The Pseudoinverse of $A = U\Sigma V^{\top} \in R^{m\times n}$:

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

$$A^+ \in R^{n \times m}$$

Motivation

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Matrix Norms

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Progrustos Problem

Pseudoinverses

Low-Rank Appro

Matrix Norm

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PCA

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

• A **overdetermined** \Rightarrow A $\stackrel{\rightarrow}{b}$ gives least-squares

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

SVD

Pseudoinverses

Low-Rank Approx.

Matrix Norms

Regularization

Procrustes Problem

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

Outer Product

Motivation

2 V D

Pseudoinverses

Low-Rank Approx.

Matrix Norms

Daniel Control

D., D., I.I.

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

Computing $A\vec{x}$

Motivation

Pseudoinverse

Low-Rank Approx.

Matrix Norms

regularization

Procrustes Problen

$$A\vec{x} = \sum_{i} \sigma_i (\vec{v_i} \cdot \vec{x}) \vec{u_i}$$

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Procrustes Probler

PCA

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

Trick:

Ignore small σ_i .

这里的small指的是乘上以后趋于0

SVD

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Matrix Norms

Damilantantian

D... D.... I.I.

PCA

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

Trick: Ignore large σ_i .

Motivation

Degudoinvorcos

Low-Rank Approx.

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Do not compute large (small) σ_i at all!

Low-Rank Approx.

Theorem

Suppose \tilde{A} is obtained from $A = U\Sigma V^{\top}$ by truncating all but the k largest singular values σ_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

Motivation

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PCA

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

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

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

Revisiting Tikhonov Regularization

Motivation

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PCA

Regularized least-squares problem:

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

Perform SVD analysis. What does α do to the singular values?

Solution:
$$\hat{x} = VDU^{\top}\vec{b}$$

$$D_{ii} = \frac{\sigma_i}{\sigma_i^2 + \alpha^2}$$

Rigid Alignment

刚体的

Procrustes Problem



Point cloud 1



Point cloud 2





Final alignment

Variational Formulation

Motivation

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Matrix Norms

Procrustes Problem

PCA

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

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

Variational Formulation

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PCA

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

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

Alternate:

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

Procrustes via SVD

Motivation

SVD

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Low-Rank Approx.

Matrix Norms

Watrix Worlds

Procrustes Problem

РСА

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

Procrustes Problem

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

Orthogonal Procrustes Theorem

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

$$YX^{+} = U\Sigma V^{+}$$
.

Application: As-Rigid-As-Possible

Motivation

Proudoinvorce

Low-Rank Appro

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PCA

As-Rigid-As-Possible Surface Modeling

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

https://igl.ethz.ch/projects/ARAP/



Related: Polar Decomposition

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PC/

$$F = RU$$

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

Motivation

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

- Age
- Weight
- Blood pressure
- Heart rate

Find: Correlations between different dimensions

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One-dimensional subspace

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

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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.

Mathematics Methods for Computer Science

Application: Eigenfaces

Motivation

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Matrix Norms

Regularizati

Procrustes Problen

PCA





(a) Input faces

(b) Eigenfaces



$$= -13.1 \times$$



(c) Projection

 $+ \cdots$

Application: CNN Fluid Simulation

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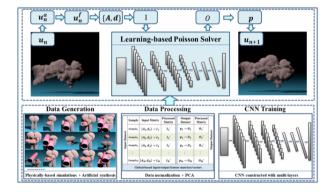
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Xiao, X., Zhou, Y., Wang, H. and Yang, X., 2020. A novel cnn-based poisson solver for fluid simulation. IEEE transactions on visualization and computer graphics, 26(3). http://dalab.se.sjtu.edu.cn/www/home/?page_id=790