Mathematics Methods for Computer Science

Instructor: Xubo Yang

SJTU-SE DALAB

Lecture

Singular Value Decomposition

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

Critical points of the ratio:

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

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

Critical points of the ratio:

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

- $R(\alpha\vec{v}) = R(\vec{v}) \Rightarrow$ take $\|\vec{v}\|_2 = 1$
- $R(\vec{v}) \geq 0 \Rightarrow$ study $R^2(\vec{v})$ instead

Once Again...

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

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

$\Rightarrow$ $\vec{v}_i$ satisfying $A^\top A\vec{v}_i = \lambda_i\vec{v}_i$

Once Again...

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

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: $A^\top A$ is symmetric positive semidefinite

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

Geometric Question

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

Geometric Question

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

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

Observation

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):

$$A^\top A\hat{v}_i = \lambda_i \hat{v}_i$$

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

$$AA^\top \vec{u}_i = \lambda_i \vec{u}_i$$

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

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

Observation

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

Lemma

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

$$
\begin{aligned}
\bar{\Sigma} &\equiv diag(\sqrt{\lambda_1}, \cdots, \sqrt{\lambda_k}) \\
&= diag(\sigma_i, \cdots, \sigma_k) (\sigma_i \text{ are singular values})
\end{aligned}
$$

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

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

Fat SVD: Completing the Basis

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

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

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

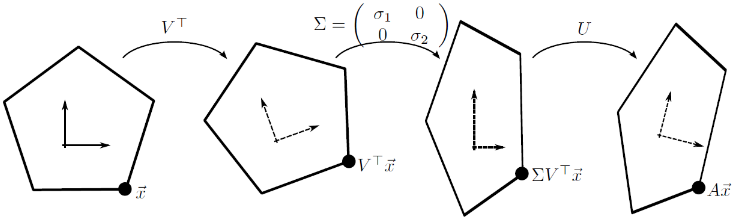
$$A = U\Sigma V^\top$$

U/V为正交矩阵，Σ是对角矩阵

Geometry of Linear Transformations

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

1. Rotate $(V^\top)$
2. Scale (Σ)
3. Rotate (U)



SVD Vocabulary

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

- **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

1. Columns of V are eigenvectors of $A^\top A$
2. $AV = U\Sigma \Rightarrow$ columns of U corresponding to nonzero singular values are normalized columns of AV
3. Remaining columns of U satisfy $AA^\top \vec{u}_i = \vec{0}$.

Computing SVD: Simple Strategy

1. Columns of V are eigenvectors of $A^\top A$
2. $AV = U\Sigma \Rightarrow$ columns of U corresponding to nonzero singular values are normalized columns of AV
3. Remaining columns of U satisfy $AA^\top \vec{u}_i = \vec{0}$.

$\exists$ **more specialized methods!**

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

$$
\begin{aligned}
A\vec{x} &= \vec{b} \\
\implies U\Sigma V^\top \vec{x} &= \vec{b} \\
\implies \qquad \vec{x} &= V\Sigma^{-1}U^\top \vec{b}
\end{aligned}
$$

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

$$
\begin{aligned}
A\vec{x} &= \vec{b} \\
\Longrightarrow U\Sigma V^\top \vec{x} &= \vec{b} \\
\Longrightarrow \quad \vec{x} &= V\Sigma^{-1}U^\top \vec{b}
\end{aligned}
$$

What is Σ^{-1} ?

为 Σ 中对角线上元素全部取倒数得到的矩阵

Uniting Short/Tall Matrices

$$\text{minimize } \|\vec{x}\|_2^2$$
$$\text{such that } A^\top A\vec{x} = A^\top \vec{b}$$

Simplification

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

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

Simplification

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

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

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

$$\vec{y} \equiv V^\top \vec{x}$$

$$\vec{d} \equiv U^\top \vec{b}$$

Resulting Optimization

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

Resulting Optimization

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

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

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

$$y_i = \begin{cases} \frac{d_i}{\sigma_i} & \sigma_i \neq 0 \\ \text{no constraint (take 0)} & \sigma_i = 0 \end{cases}$$

Solution

$$\Sigma^+_{ij} \equiv \begin{cases} 1/\sigma_i & i = j, \sigma_i \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

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

Pseudoinverse

矩阵A^+称为矩阵A的伪逆矩阵

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

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

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

Pseudoinverse Properties

- A **square** and **invertible** $\Rightarrow A^+ = A^{-1}$
- A **overdetermined** $\Rightarrow A^+\vec{b}$ gives least-squares
- A **underdetermined** $\Rightarrow A^+\vec{b}$ gives least-squares solution to $A\vec{x} \approx \vec{b}$ with least (Euclidean) norm

Alternative Form

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

Outer Product

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

Computing $A\vec{x}$

$$A\vec{x} = \sum_i \sigma_i \underbrace{(\vec{v}_i \cdot \vec{x})}_{\text{是一个标量}} \vec{u}_i$$

Computing $A\vec{x}$

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

Trick:

Ignore small σ_i.

这里的small指的是乘上以后趋于0

Computing $A^+\vec{x}$

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

Trick:

Ignore large σ_i.

Even Better Trick

Do not compute large (small) σ_i at all!

Eckart-Young Theorem

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

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

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

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

Revisiting Tikhonov Regularization

Regularized least-squares problem:
$(A^\top A + \alpha I)\vec{x} = A^\top \vec{b}$.

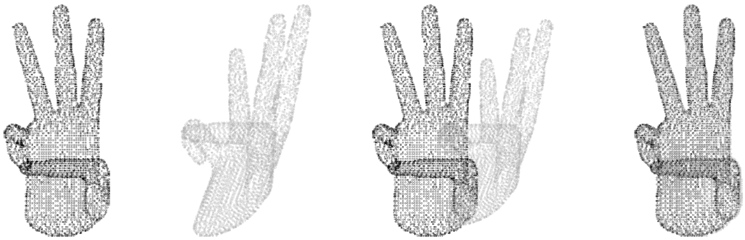
Perform SVD analysis.
What does α do to the singular values?

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

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

Rigid Alignment

刚体的



Point cloud 1 Point cloud 2 Initial alignment Final alignment

Variational Formulation

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

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:

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

Procrustes via SVD

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

Procrustes via SVD

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

Orthogonal Procrustes Theorem

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

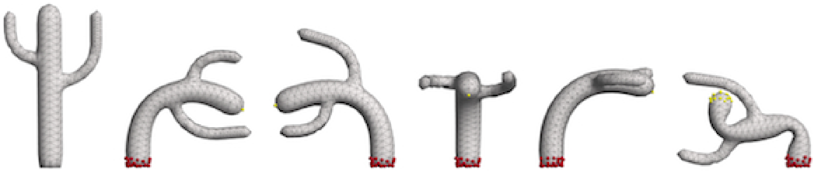
Application: As-Rigid-As-Possible

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

$$F = RU$$

Special case:

- F is square real-valued matrix;
- R is best rotation matrix approximation;
- 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

Simplest Model

One-dimensional subspace

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

More General Statement

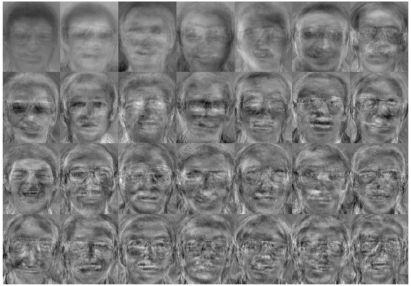
Principal Component Analysis

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 $X = U\Sigma V^\top$.

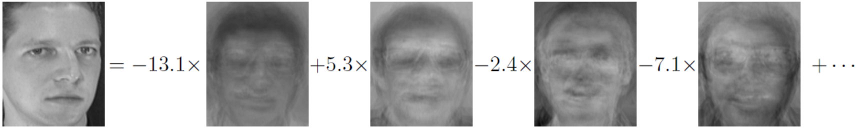
Proved in textbook.

Application: Eigenfaces

(a) Input faces

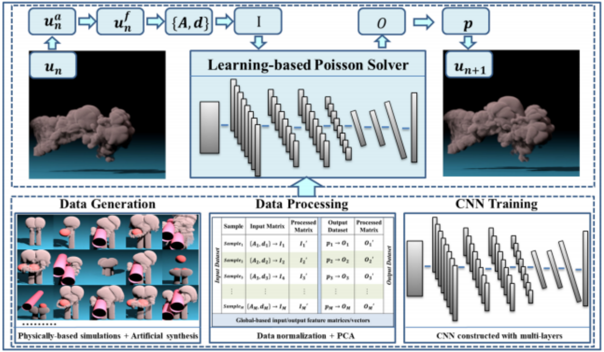


(b) Eigenfaces



(c) Projection

Application: CNN Fluid Simulation



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