PCA

SVD

Singular Value Decomposition

CS 205A:

Mathematical Methods for Robotics, Vision, and Graphics

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Understanding the Geometry of

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

Critical points of the ratio:

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

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Critical points of the ratio:

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

- $R(\alpha \vec{x}) = R(\vec{x}) \implies \mathsf{take} \ \|\vec{x}\|_2 = 1$
- $ightharpoonup R(\vec{x}) \geq 0 \implies \text{study } R^2(\vec{x}) \text{ instead}$



Once Again...

Critical points satisfy

$$A^{\top} A \vec{x}_i = \lambda_i \vec{x}_i$$



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Properties:

$$\lambda_i \geq 0 \, \forall i$$

Once Again...

Critical points satisfy

$$A^{\top} A \vec{x}_i = \lambda_i \vec{x}_i$$

Properties:

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



Geometric Question

How is \vec{x}_i related to the geometry of A rather than that of $A^{\top}A$?



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How is \vec{x}_i related to the geometry of A rather than that of $A^{\top}A$?

Object of study: $\vec{y_i} = A\vec{x_i}$

Observation

Lemma

Either $\vec{y}_i = \vec{0}$ or \vec{y}_i is an eigenvector of AA^{\top} with $\|\vec{y}_i\| = \sqrt{\lambda_i} \|\vec{x}_i\|$.

Corresponding Eigenvalues

$$k = \text{ number of } \lambda_i > 0$$

$$A^{\top} A \vec{x}_i = \lambda_i \vec{x}_i$$

$$A A^{\top} \vec{y}_i = \lambda_i \vec{y}_i$$

$$\bar{U} \in \mathbb{R}^{n \times k} = \text{ matrix of } \vec{x}_i \text{'s}$$

$$\bar{V} \in \mathbb{R}^{m \times k} = \text{ matrix of } \vec{y}_i \text{'s}$$

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Lemma

$$\bar{U}^{\top} A \bar{V} \vec{e_i} = \sqrt{\lambda_i} \vec{e_i}$$



Observation

Lemma

$$\bar{U}^{\top} A \bar{V} \vec{e_i} = \sqrt{\lambda_i} \vec{e_i}$$

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



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Lemma

$$\bar{U}^{\top} A \bar{V} \vec{e_i} = \sqrt{\lambda_i} \vec{e_i}$$

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

Corollary

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



Add
$$\vec{x}_i$$
 with $A^{\top}A\vec{x}_i = \vec{0}$ and \vec{y}_i with $AA^{\top}\vec{y}_i = \vec{0}$

Completing the Basis

Add \vec{x}_i with $A^{\top}A\vec{x}_i = \vec{0}$ and \vec{y}_i with $AA^{\top}\vec{y}_i = \vec{0}$

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



SVD

Completing the Basis

Add \vec{x}_i with $A^{\top}A\vec{x}_i=\vec{0}$ and \vec{y}_i with $AA^{\top}\vec{y}_i=\vec{0}$

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



Singular Value Decomposition



Motivation

SVD Vocabulary

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

- Left singular vectors: Columns of U; span $\operatorname{col} A$
- ▶ Right singular vectors Columns of V; span row A
- ▶ Singular values: Diagonal σ_i of Σ ; sort $\sigma_1 > \sigma_2 > \cdots > 0$.



Motivation 000000

SVD

Geometry of Linear Transformations

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

- **1.** Rotate (V^{\top})
 - **2.** Scale (Σ)
 - 3. Rotate (U)



Computing SVD: Simple Strategy

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

Motivation

SVD

Computing SVD: Simple Strategy

- **1.** Columns of V are eigenvectors of $A^{T}A$
- 2. $AV = U\Sigma \implies \text{columns of } U$ corresponding to nonzero singular values are normalized columns of AV
- **3.** Remaining columns of U satisfy $AA^{\dagger}\vec{u}_i = 0$.
 - ∃ more specialized methods!



Solving Linear Systems with

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

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

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

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

SVD

Solving Linear Systems with

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

What is Σ^{-1} ?



SVD

Uniting Short/Tall Matrices

minimize
$$\|\vec{x}\|_2^2$$

such that $A^{\top}A\vec{x} = A^{\top}\vec{b}$

Simplification

$$A^{\top}A = V\Sigma^2 V^{\top}$$

Simplification

$$A^{\top}A = V\Sigma^2 V^{\top}$$

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



SVD

Resulting Optimization

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



Solution

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

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

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

Pseudoinverse

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

Pseudoinverse Properties

- A square and invertible $\implies A^+ = A^{-1}$
- A overdetermined $\implies A^+ \vec{b}$ gives least-squares solution to $A \vec{x} \approx \vec{b}$
- A underdetermined $\implies A^+ \vec{b}$ 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 $A\vec{x}$

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

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Trick: Ignore small σ_i .



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 $\|A - \tilde{A}\|_{\operatorname{Fro}}$ and $\|A - \tilde{A}\|_2$ subject to the constraint that the column space of \tilde{A} has at most dimension k.

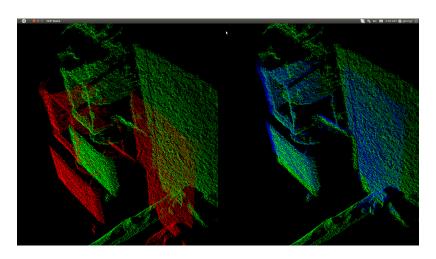


Matrix Norm Expressions

$$||A||_{\text{Fro}}^2 = \sum_{j} \sigma_j^2$$

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

$$\operatorname{cond} A = \frac{\sigma_{\max}}{\sigma_{\min}}$$



http://www.pointclouds.org/blog/_images/GICPRegistrationTopView.png



Motivation

SVD

Procrustes Problem

Procrustes

From Wikipedia, the free encyclopedia

"Damastes" redirects here. For the spider genus, see Damastes (spider).

For the Larry Niven story, see Procrustes (short story).

In Greek mythology, Procrustes (Προκρούστης) or "the stretcher [who hammers out the metal]", also known as Prokoptas or Damastes (Δαμαστής) "subduer", was a rogue smith and bandit from Attica who physically attacked people by stretching them or cutting off their legs, so as to force them to fit the size of an iron bed. In general, when something is Procrustean, different lengths or sizes or properties are fitted to an arbitrary standard.

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http://en.wikipedia.org/wiki/Procrustes

Procrustes via SVD

Orthogonal Procrustes Theorem

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

Proved in notes.



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



Motivation

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 Components Analysis

The matrix $C \in \mathbb{R}^{n \times d}$ minimizing $\|X - CC^{\top}X\|_{\text{Fro}}$ 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 notes.



