Lecture 12: SVD, Procrustes Analysis

COMPSCI/MATH 290-04

Chris Tralie, Duke University

2/23/2016

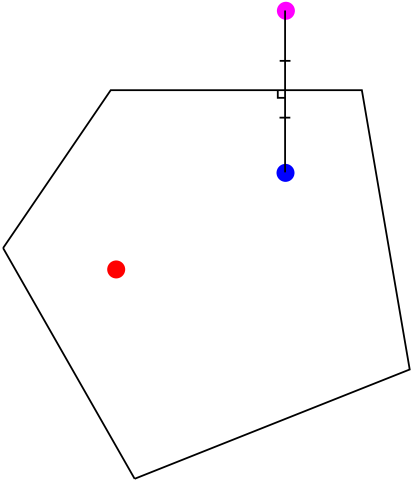
Announcements

- Group Assignment 1 Full Submission Due next Tuesday 11:55 PM
- Hackathon Saturday 2/27 4:00 PM - 10:00 PM Gross Hall 330
- Rank Top 3 Final Project Choices By Next Wednesday 3/2

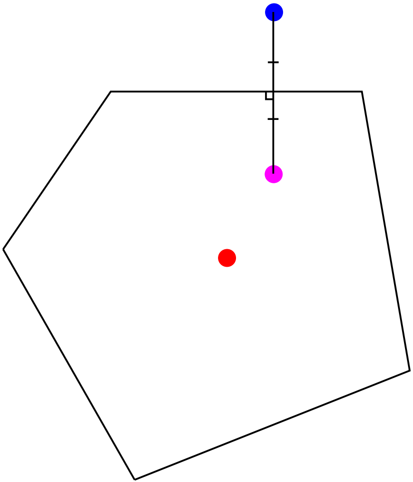
Table of Contents

- ▶ Ray Tracing Special Case
- ▷ PCA Review
- ▷ Singular Value Decomposition
- ▷ Procrustes Distance
- ▷ Final Projects

Ray Tracing Special Case



Ray Tracing Special Case



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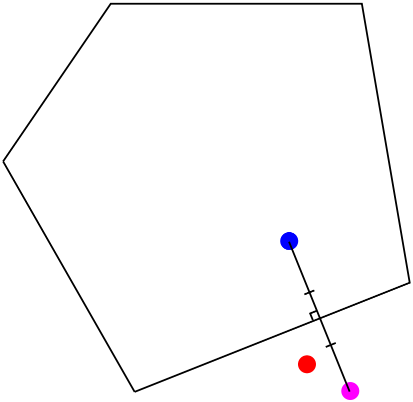

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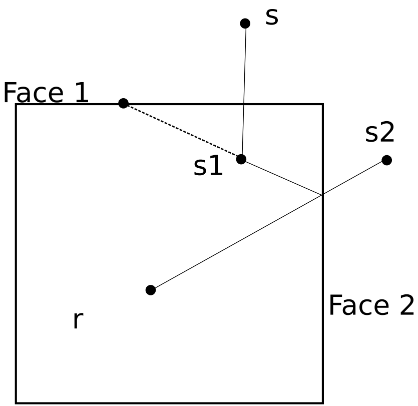

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PCA Review

Organize point cloud into $N \times d$ matrix, each point *along a column*

$$X = \begin{bmatrix} | & | & \cdots & | \\ \vec{v_1} & \vec{v_2} & \vdots & \vec{v_N} \\ | & | & \cdots & | \end{bmatrix}$$

Choose a unit column vector direction $u \in \mathbb{R}^{d \times 1}$
Then

$$d = u^T X$$

gives projections onto u

PCA Review

Organize point cloud into $N \times d$ matrix, each point *along a column*

$$X = \begin{bmatrix} | & | & \cdots & | \\ \vec{v}_1 & \vec{v}_2 & \vdots & \vec{v}_N \\ | & | & \cdots & | \end{bmatrix}$$

Choose a unit column vector direction $u \in \mathbb{R}^{d \times 1}$
Then

$$d = u^T X$$

gives projections onto u

- More consistent with what we've done; points in columns

PCA New Convention

$$d = u^T X$$

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- How to express the sum of the squares of the dot products?

PCA New Convention

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$$dd^T$$

PCA New Convention

$$d = u^T X$$

- How to express the sum of the squares of the dot products?

$$dd^T$$

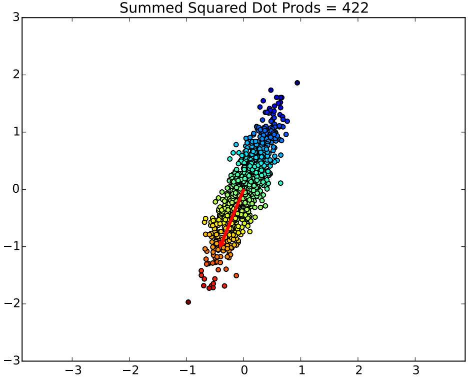
$$dd^T = (u^T X)(u^T X)^T = u^T X X^T u$$

Want to find u that maximizes the above quadratic form

PCA New Convention

Use eigenvectors of $A = XX^T$ to find principal directions maximizing $u^T A u$

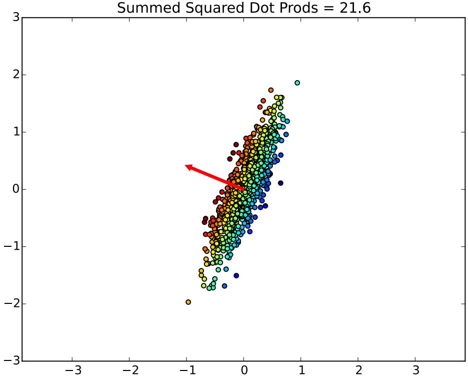
$$\lambda_1 = 422$$



PCA Review

Use eigenvectors of $A = XX^T$ to find principal directions maximizing $u^T Au$

$$\lambda_2 = 21.6$$



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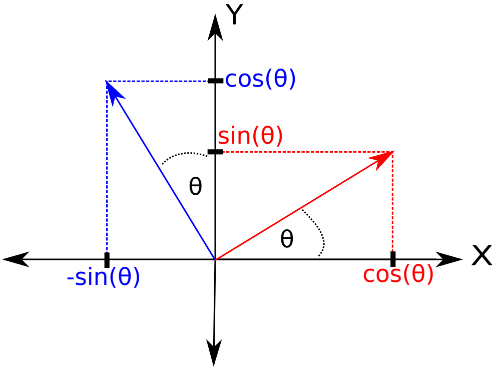
Orthogonal Matrices / Rotation Review

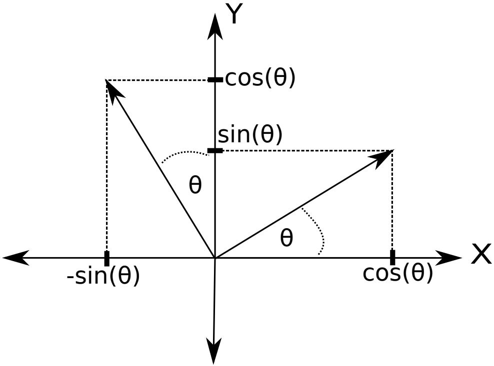
$$\begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$



Orthogonal Matrices / Rotation Review

Inverse rotation: dot product interpretation

$$\begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$



Orthogonal Matrices / Rotation Review

In general

$$R = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_N} \\ | & | & \vdots & | \end{bmatrix}$$

$$\vec{u_i} \cdot \vec{u_j} = 1, i = j$$

$$\vec{u_i} \cdot \vec{u_j} = 0, i \neq j$$

In 3D,

$$\vec{u_1} \times \vec{u_2} = \vec{u_3}$$

for a pure rotation

Orthogonal Matrices / Rotation Review

$$R = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_N} \\ | & | & \vdots & | \end{bmatrix}$$

$$R^T = \begin{bmatrix} - & \vec{u_1} & - \\ - & \vec{u_2} & - \\ \dots & \vdots & \dots \\ - & \vec{u_N} & - \end{bmatrix}$$

$$\vec{u_i} \cdot \vec{u_j} = 1, i = j$$

$$\vec{u_i} \cdot \vec{u_j} = 0, i \neq j$$

$$R^T R = R R^T = I$$

Singular Value Decomposition

Given an $m \times n$ matrix A, the SVD of A is

$$A = USV^T$$

- U is an $M \times M$ rotation matrix
- S is an $M \times N$ matrix, where $S_{ij} = 0 \; i \neq j$
- V is an $N \times N$ rotation matrix

$$A = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_M} \\ | & | & \vdots & | \end{bmatrix} \begin{bmatrix} s_1 & 0 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ 0 & 0 & s_3 & \dots & 0 \\ \dots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & s_M & \dots 0 \end{bmatrix} \begin{bmatrix} - & \vec{v_1} & - \\ - & \vec{v_2} & - \\ \dots & \vdots & \dots \\ - & \vec{v_N} & - \end{bmatrix}$$

Singular Value Decomposition

$$A = USV^T$$

$$A = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_M} \\ | & | & \vdots & | \end{bmatrix} \begin{bmatrix} s_1 & 0 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ 0 & 0 & s_3 & \dots & 0 \\ \dots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & s_M & \dots 0 \end{bmatrix} \begin{bmatrix} - & \vec{v_1} & - \\ - & \vec{v_2} & - \\ \dots & \vdots & \dots \\ - & \vec{v_N} & - \end{bmatrix}$$

Singular Value Decomposition

$$A = USV^T$$

$$A = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_M} \\ | & | & \vdots & | \end{bmatrix} \begin{bmatrix} s_1 & 0 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ 0 & 0 & s_3 & \dots & 0 \\ \dots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & s_M & \dots 0 \end{bmatrix} \begin{bmatrix} - & \vec{v_1} & - \\ - & \vec{v_2} & - \\ \dots & \vdots & \dots \\ - & \vec{v_N} & - \end{bmatrix}$$

- $s_1 > s_2 > s_3 > ... > s_M$

Singular Value Decomposition

$$A = USV^T$$

$$A = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_M} \\ | & | & \vdots & | \end{bmatrix} \begin{bmatrix} s_1 & 0 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ 0 & 0 & s_3 & \dots & 0 \\ \dots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & s_M & \dots 0 \end{bmatrix} \begin{bmatrix} - & \vec{v_1} & - \\ - & \vec{v_2} & - \\ \dots & \vdots & \dots \\ - & \vec{v_N} & - \end{bmatrix}$$

- $s_1 > s_2 > s_3 > ... > s_M$
- U holds the eigenvectors of AA^T

Singular Value Decomposition

$$A = USV^T$$

$$A = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_M} \\ | & | & \vdots & | \end{bmatrix} \begin{bmatrix} s_1 & 0 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ 0 & 0 & s_3 & \dots & 0 \\ \dots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & s_M & \dots 0 \end{bmatrix} \begin{bmatrix} - & \vec{v_1} & - \\ - & \vec{v_2} & - \\ \dots & \vdots & \dots \\ - & \vec{v_N} & - \end{bmatrix}$$

- $s_1 > s_2 > s_3 > ... > s_M$
- U holds the eigenvectors of AA^T
- V holds the eigenvectors of $A^T A$

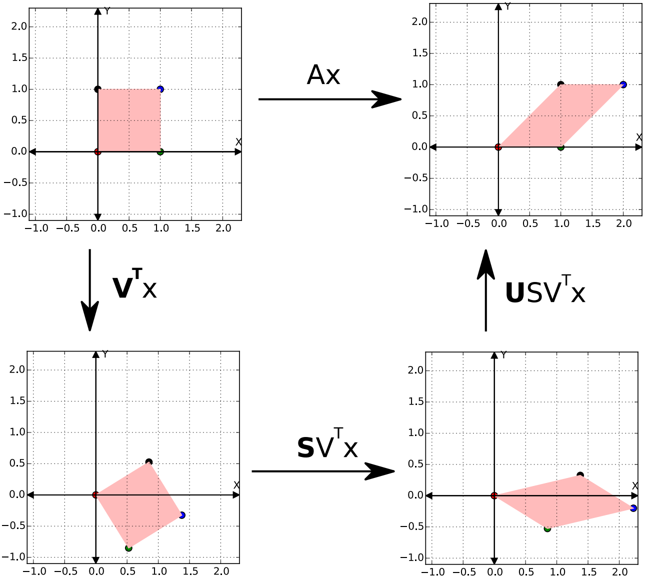
Singular Value Decomposition

$$A = USV^T$$

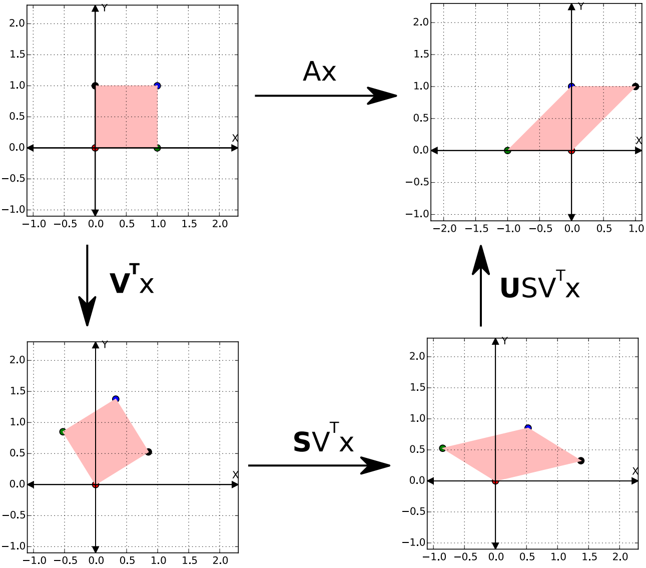
$$A = \begin{bmatrix} | & | & \vdots & | \\ \vec{u_1} & \vec{u_2} & \dots & \vec{u_M} \\ | & | & \vdots & | \end{bmatrix} \begin{bmatrix} s_1 & 0 & 0 & \dots & 0 \\ 0 & s_2 & 0 & \dots & 0 \\ 0 & 0 & s_3 & \dots & 0 \\ \dots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & s_M & \dots 0 \end{bmatrix} \begin{bmatrix} - & \vec{v_1} & - \\ - & \vec{v_2} & - \\ \dots & \vdots & \dots \\ - & \vec{v_N} & - \end{bmatrix}$$

- $s_1 > s_2 > s_3 > ... > s_M$
- U holds the eigenvectors of AA^T
- V holds the eigenvectors of A^TA
- Each s is the square root of corresponding eigenvalue of AA^T and A^TA (they're the same!)

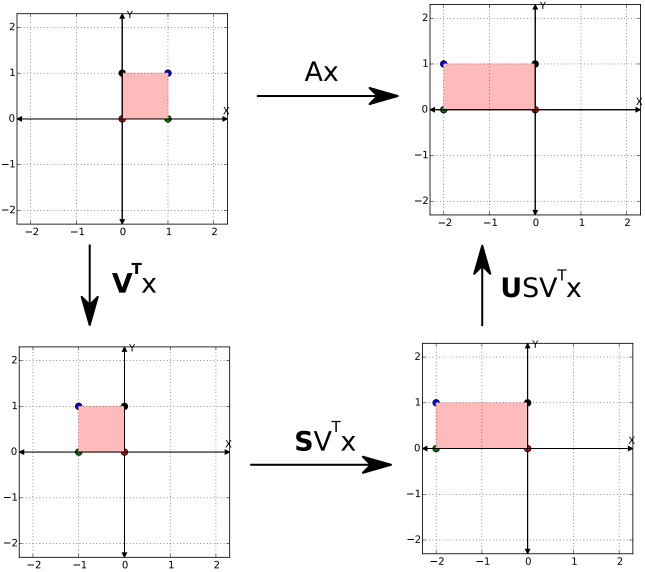
Singular Value Decomposition: Example



Singular Value Decomposition: Example



Singular Value Decomposition: Example



Singular Value Decomposition $\rightarrow$ PCA

$$A = USV^T$$

- $s_1 > s_2 > s_3 > ... > s_M$
- U holds the eigenvectors of AA^T
- V holds the eigenvectors of $A^T A$
- Each s is the square root of corresponding eigenvalue of AA^T and $A^T A$

Let X be a $3 \times N$ matrix of points along columns.
Can we use SVD(X) to do PCA?

Singular Value Decomposition → PCA

$$X = USV^T$$

- Columns of U give principal components
- Squares of corresponding S gives sum of squared magnitudes along directions of U
- Coordinates along U directions?

Table of Contents

▷ Ray Tracing Special Case

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▷ Singular Value Decomposition

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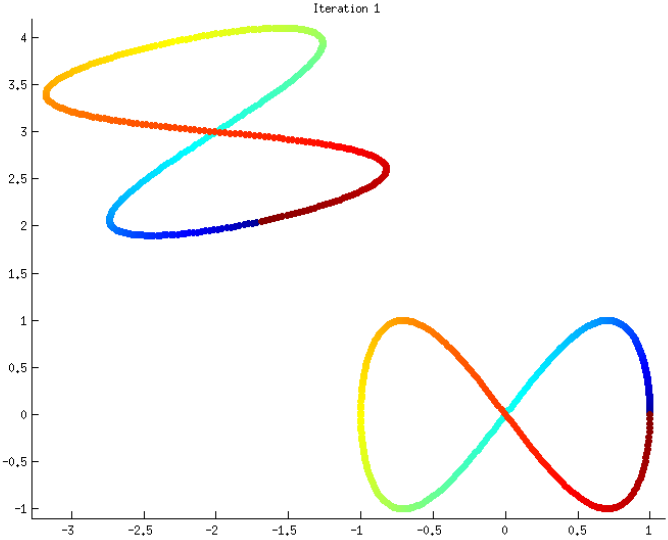
Procrustes Distance

http://www.procrustes.nl/gif/illustr.gif

Procrustes Alignment



Procrustes Distance

Given two point clouds $\{\vec{x}_i\}_{i=1}^N$ and $\{\vec{y}_i\}_{i=1}^N$
where x_i and y_i are in correspondence
Seek to minimize

$$\sum_{i=1}^{N} ||R(\vec{x}_i + \vec{t}) - \vec{y}_i||_2^2$$

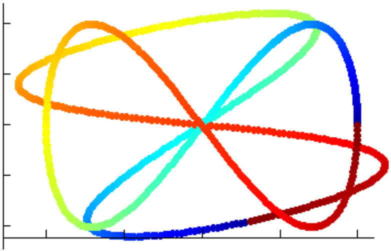
over all orthogonal matrices R and translation vectors t. $||.||_2^2$ is squared distance

Translation

$$\sum_{i=1}^{N} ||R(\vec{x}_i + \vec{t}) - \vec{y}_i||_2^2$$

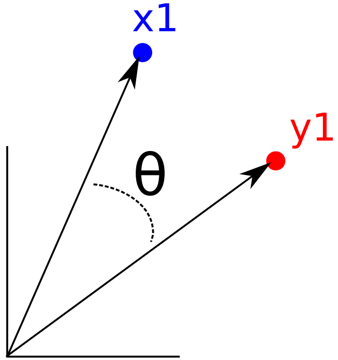
Translation is easy! Align centroids

$$\vec{t} = \frac{1}{N}\left(\sum_{i=1}^{N} \vec{y}_i - \sum_{i=1}^{N} \vec{x}_i\right)$$



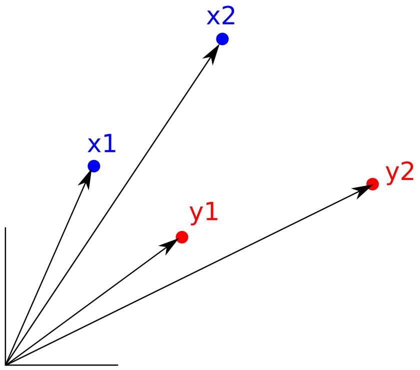
Rotating to Align Points: Dot Product Perspective

$$\vec{x_1} \cdot \vec{y_1} = ||\vec{x_1}||||\vec{y_1}|| \cos(\theta_1)$$



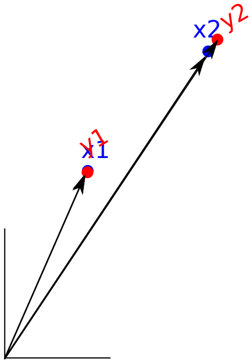
Rotating to Align Points: Dot Product Perspective

$$\vec{x_1} \cdot \vec{y_1} + \vec{x_2} \cdot \vec{y_2} = ||\vec{x_1}||||\vec{y_1}|| \cos(\theta_1) + ||\vec{x_2}||||\vec{y_2}|| \cos(\theta_2)$$



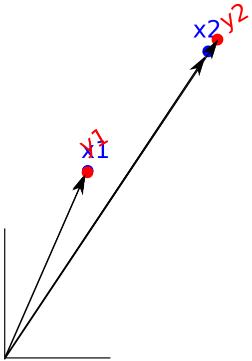
Rotating to Align Points: Dot Product Perspective

$$\vec{x_1} \cdot \vec{y_1} + \vec{x_2} \cdot \vec{y_2} = ||\vec{x_1}||||\vec{y_1}|| \cos(\theta_1) + ||\vec{x_2}||||\vec{y_2}|| \cos(\theta_2)$$



Rotating to Align Points: Dot Product Perspective

$$\vec{x_1} \cdot \vec{y_1} + \vec{x_2} \cdot \vec{y_2} = ||\vec{x_1}||||\vec{y_1}|| \cos(\theta_1) + ||\vec{x_2}||||\vec{y_2}|| \cos(\theta_2)$$

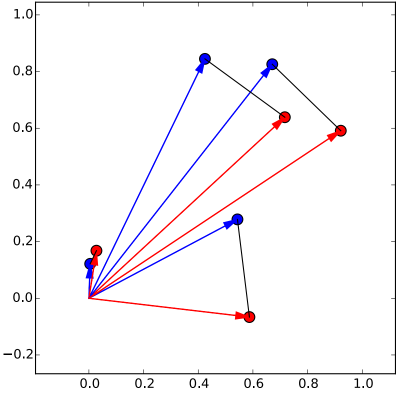


- Why should points further away from origin get more weight?

Rotating to Align Points: Dot Product Perspective

In general, how to maximize?

$$\sum_{i=1}^{N} R_x \vec{x}_i \cdot R_y \vec{y}_i$$



Rotating to Align Points: Dot Product Perspective

In general, how to maximize?

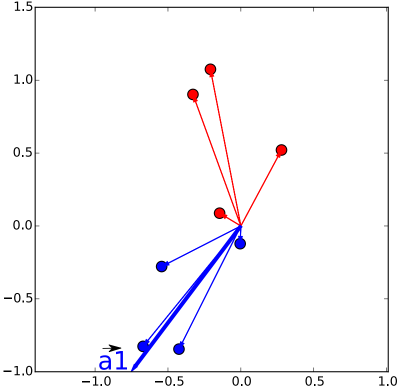
$$\sum_{i=1}^{N} R_x \vec{x}_i \cdot R_y \vec{y}_i$$

VIDEO EXAMPLE

Maximizing Dot Product: First Component

Choose first row of R_x, which is a projection of blue points. Call this row a_1 (write as a row vector)

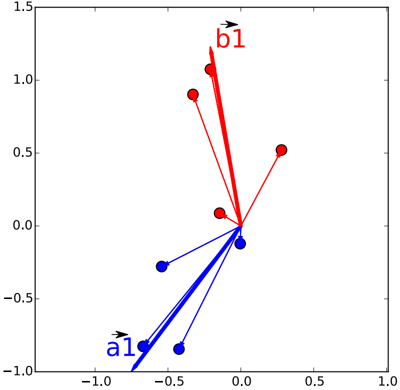
$$a_1 X$$



Maximizing Dot Product: First Component

Choose first row of Ry, which is a projection of red points. Call this row b_1 (write as row vector)

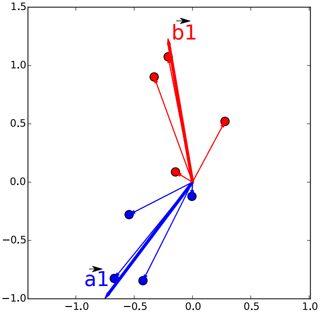
$$b_1 Y$$



Maximizing Dot Product: First Component

$$a_1 X, b_1 Y$$

How to write $\sum_{i=1}^{N} (\vec{a_1} \cdot \vec{x_i})(\vec{b_1} \cdot \vec{y_i})$ in matrix form?

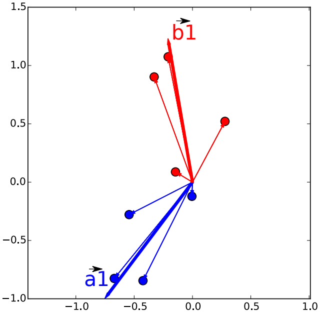


Maximizing Dot Product: First Component

$$a_1 X, b_1 Y$$

How to write $\sum_{i=1}^{N} (\vec{a_1} \cdot \vec{x_i})(\vec{b_1} \cdot \vec{y_i})$ in matrix form?

$$(a_1 X)(b_1 Y)^T = a_1 X Y^T b_1^T$$



Maximizing Dot Product: First Component

How to find u_1 and v_1 that maximize this product?

$$(a_1 X)(b_1 Y)^T = a_1 XY^T b_1^T$$

Take SVD: $XY^T = USV^T$ and substitute in

$$a_1 USV^T b_1^T$$

Continued next time...