Introduction to Machine Learning

Feature Generation

Andres Mendez-Vazquez

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Outline

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What do we want?

What

- Given a set of measurements, the goal is to discover compact and informative representations of the obtained data.

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Our Approach

- We want to “squeeze” in a relatively small number of features, leading to a reduction of the necessary feature space dimension.

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Our Approach

- We want to "squeeze" in a relatively small number of features, leading to a reduction of the necessary feature space dimension.

Properties

- Thus removing information redundancies - Usually produced and the measurement.

What Methods we will see?

Fisher Linear Discriminant

1. Squeezing to the maximum.
2. From Many to One Dimension

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Principal Component Analysis

1. Not so much squeezing
2. You are willing to lose some information

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Rotation

Projecting

Projecting well-separated samples onto an arbitrary line usually produces a confused mixture of samples from all of the classes and thus produces poor recognition performance.

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Something Notable

However, moving and rotating the line around might result in an orientation for which the projected samples are well separated.

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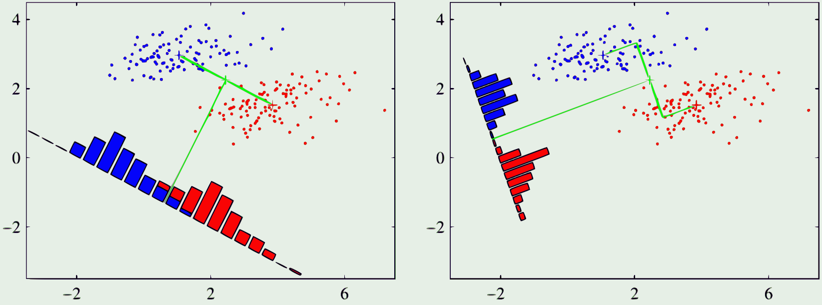
Fisher linear discriminant (FLD)

It is a discriminant analysis seeking directions that are efficient for discriminating binary classification problem.

Example

Example - From Left to Right the Improvement



This is actually comming from...

Classifier as

A machine for dimensionality reduction.

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Initial Setup

We have:

- N d-dimensional samples $x_1, x_2, ..., x_N$
- N_i is the number of samples in class C_i for i=1,2.

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Initial Setup

We have:

- N d-dimensional samples $x_1, x_2, ..., x_N$
- N_i is the number of samples in class C_i for i=1,2.

Then, we ask for the projection of each x_i into the line by means of

$$y_i = \boldsymbol{w}^T \boldsymbol{x}_i \tag{1}$$

Outline

Use the mean of each Class

Then

Select $\boldsymbol{w}$ such that class separation is maximized

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Select $\boldsymbol{w}$ such that class separation is maximized

We then define the mean sample for ecah class

1. $C_1 \Rightarrow \boldsymbol{m}_1 = \frac{1}{N_1}\sum_{i=1}^{N_1} \boldsymbol{x}_i$
2. $C_2 \Rightarrow \boldsymbol{m}_2 = \frac{1}{N_2}\sum_{i=1}^{N_2} \boldsymbol{x}_i$

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Ok!!! This is giving us a measure of distance

Thus, we want to maximize the distance the projected means:

$$m_1 - m_2 = \boldsymbol{w}^T (\boldsymbol{m}_1 - \boldsymbol{m}_2) \quad (2)$$

where $m_k = \boldsymbol{w}^T \boldsymbol{m}_k$ for $k = 1, 2$.

However

We could simply seek

$$\max \boldsymbol{w}^T (\boldsymbol{m}_1 - \boldsymbol{m}_2)$$
$$s.t. \sum_{i=1}^{d} w_i = 1$$

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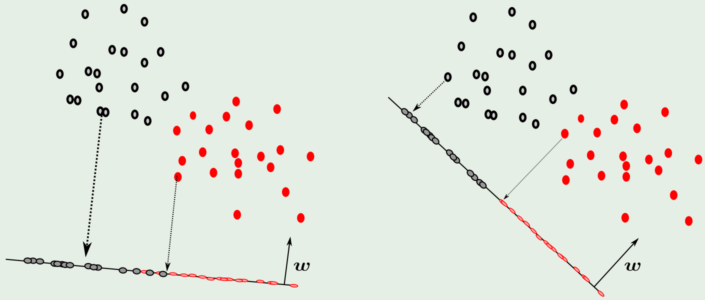
After all

We do not care about the magnitude of $\boldsymbol{w}$.

Example

Here, we have the problem



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Fixing the Problem

To obtain good separation of the projected data

The difference between the means should be large relative to some measure of the standard deviations for each class.

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We define a SCATTER measure (Based in the Sample Variance)

$$s_k^2 = \sum_{\boldsymbol{x}_i \in C_k} \left(\boldsymbol{w}^T \boldsymbol{x}_i - m_k \right)^2 = \sum_{y_i = \boldsymbol{w}^T \boldsymbol{x}_i \in C_k} \left(y_i - m_k \right)^2 \quad (3)$$

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We define then within-class variance for the whole data

$$s_1^2 + s_2^2 \tag{4}$$

Outline

Finally, a Cost Function

The between-class variance

$$(m_1 - m_2)^2 \tag{5}$$

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The Fisher criterion

$$\frac{\text{between-class variance}}{\text{within-class variance}} \tag{6}$$

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Finally

$$J(\boldsymbol{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2} \tag{7}$$

We use a transformation to simplify our life

First

$$J(\boldsymbol{w}) = \frac{\left(\boldsymbol{w}^T\boldsymbol{m}_1 - \boldsymbol{w}^T\boldsymbol{m}_2\right)^2}{\sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_1}(y_i - m_k)^2 + \sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_2}(y_i - m_k)^2}$$

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Second

$$= \frac{\left(\boldsymbol{w}^T\boldsymbol{m}_1 - \boldsymbol{w}^T\boldsymbol{m}_2\right)\left(\boldsymbol{w}^T\boldsymbol{m}_1 - \boldsymbol{w}^T\boldsymbol{m}_2\right)^T}{\sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_1}\left(\boldsymbol{w}^T\boldsymbol{x}_i - m_k\right)\left(\boldsymbol{w}^T\boldsymbol{x}_i - m_k\right)^T + \sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_2}\left(\boldsymbol{w}^T\boldsymbol{x}_i - m_k\right)\left(\boldsymbol{w}^T\boldsymbol{x}_i - m_k\right)^T}$$

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Third

$$= \frac{\boldsymbol{w}^T(\boldsymbol{m}_1 - \boldsymbol{m}_2)\left(\boldsymbol{w}^T(\boldsymbol{m}_1 - \boldsymbol{m}_2)\right)^T}{\sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_1}\boldsymbol{w}^T(\boldsymbol{x}_i - \boldsymbol{m}_1)\left(\boldsymbol{w}^T(\boldsymbol{x}_i - \boldsymbol{m}_1)\right)^T + \sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_2}\boldsymbol{w}^T(\boldsymbol{x}_i - \boldsymbol{m}_2)\left(\boldsymbol{w}^T(\boldsymbol{x}_i - \boldsymbol{m}_2)\right)^T}$$

Transformation

Fourth

$$= \frac{\boldsymbol{w}^T (\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{w}}{\sum_{y_i = \boldsymbol{w}^T \boldsymbol{x}_i \in C_1} \boldsymbol{w}^T (\boldsymbol{x}_i - \boldsymbol{m}_1)(\boldsymbol{x}_i - \boldsymbol{m}_1)^T \boldsymbol{w} + \sum_{y_i = \boldsymbol{w}^T \boldsymbol{x}_i \in C_2} \boldsymbol{w}^T (\boldsymbol{x}_i - \boldsymbol{m}_2)(\boldsymbol{x}_i - \boldsymbol{m}_2)^T \boldsymbol{w}}$$

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Fifth

$$= \frac{\boldsymbol{w}^T\left(\boldsymbol{m}_1 - \boldsymbol{m}_2\right)\left(\boldsymbol{m}_1 - \boldsymbol{m}_2\right)^T\boldsymbol{w}}{\boldsymbol{w}^T\left[\sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_1}\left(\boldsymbol{x}_i - \boldsymbol{m}_1\right)\left(\boldsymbol{x}_i - \boldsymbol{m}_1\right)^T + \sum_{y_i=\boldsymbol{w}^T\boldsymbol{x}_i\in C_2}\left(\boldsymbol{x}_i - \boldsymbol{m}_2\right)\left(\boldsymbol{x}_i - \boldsymbol{m}_2\right)^T\right]\boldsymbol{w}}$$

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Now Rename

$$J\left(\boldsymbol{w}\right)=\frac{\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w}}{\boldsymbol{w}^T\boldsymbol{S}_w\boldsymbol{w}} \tag{8}$$

Derive with respect to $\boldsymbol{w}$

Thus

$$\frac{dJ\left(\boldsymbol{w}\right)}{d\boldsymbol{w}} = \frac{d\left(\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w}\right)\left(\boldsymbol{w}^T\boldsymbol{S}_w\boldsymbol{w}\right)^{-1}}{d\boldsymbol{w}} = 0 \tag{9}$$

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Then

$$\frac{dJ\left(\boldsymbol{w}\right)}{d\boldsymbol{w}}=\left(\boldsymbol{S}_{B}\boldsymbol{w}+\boldsymbol{S}_{B}^{T}w\right)\left(\boldsymbol{w}^{T}\boldsymbol{S}_{w}\boldsymbol{w}\right)^{-1}-\left(\boldsymbol{w}^{T}\boldsymbol{S}_{B}\boldsymbol{w}\right)\left(\boldsymbol{w}^{T}\boldsymbol{S}_{w}\boldsymbol{w}\right)^{-2}\left(\boldsymbol{S}_{w}\boldsymbol{w}+\boldsymbol{S}_{w}^{T}w\right)=0 \tag{10}$$

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Then

$$\frac{dJ\left(\boldsymbol{w}\right)}{d\boldsymbol{w}} = \left(\boldsymbol{S}_{B}\boldsymbol{w} + \boldsymbol{S}_{B}^{T}w\right)\left(\boldsymbol{w}^{T}\boldsymbol{S}_{w}\boldsymbol{w}\right)^{-1} - \left(\boldsymbol{w}^{T}\boldsymbol{S}_{B}\boldsymbol{w}\right)\left(\boldsymbol{w}^{T}\boldsymbol{S}_{w}\boldsymbol{w}\right)^{-2}\left(\boldsymbol{S}_{w}\boldsymbol{w} + \boldsymbol{S}_{w}^{T}w\right) = 0 \tag{10}$$

Now because the symmetry in $\boldsymbol{S}_B$ and $\boldsymbol{S}_w$

$$\frac{dJ\left(\boldsymbol{w}\right)}{d\boldsymbol{w}} = \frac{\boldsymbol{S}_{B}\boldsymbol{w}}{\left(\boldsymbol{w}^{T}\boldsymbol{S}_{w}\boldsymbol{w}\right)} - \frac{\boldsymbol{w}^{T}\boldsymbol{S}_{B}\boldsymbol{w}\boldsymbol{S}_{w}\boldsymbol{w}}{\left(\boldsymbol{w}^{T}\boldsymbol{S}_{w}\boldsymbol{w}\right)^{2}} = 0 \tag{11}$$

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Derive with respect to $\boldsymbol{w}$

Thus

$$\frac{dJ(\boldsymbol{w})}{d\boldsymbol{w}} = \frac{\boldsymbol{S}_B \boldsymbol{w}}{(\boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w})} - \frac{\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w} \boldsymbol{S}_w \boldsymbol{w}}{(\boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w})^2} = 0 \tag{12}$$

Then

$$\left(\boldsymbol{w}^T \boldsymbol{S}_w \boldsymbol{w}\right) \boldsymbol{S}_B \boldsymbol{w} = \left(\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w}\right) \boldsymbol{S}_w \boldsymbol{w} \tag{13}$$

Now, Several Tricks!!!

First

$$\boldsymbol{S}_B \boldsymbol{w} = (\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{w} = \alpha (\boldsymbol{m}_1 - \boldsymbol{m}_2) \quad (14)$$

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Where $\alpha = (\boldsymbol{m}_1 - \boldsymbol{m}_2)^T \boldsymbol{w}$ is a simple constant

It means that $\boldsymbol{S}_B\boldsymbol{w}$ is always in the direction $\boldsymbol{m}_1 - \boldsymbol{m}_2$!!!

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It means that $\boldsymbol{S}_B\boldsymbol{w}$ is always in the direction $\boldsymbol{m}_1 - \boldsymbol{m}_2$!!!

In addition

$\boldsymbol{w}^T\boldsymbol{S}_w\boldsymbol{w}$ and $\boldsymbol{w}^T\boldsymbol{S}_B\boldsymbol{w}$ are constants

Now, Several Tricks!!!

Finally

$$\boldsymbol{S}_w \boldsymbol{w} \propto (\boldsymbol{m}_1 - \boldsymbol{m}_2) \Rightarrow \boldsymbol{w} \propto \boldsymbol{S}_w^{-1} (\boldsymbol{m}_1 - \boldsymbol{m}_2) \tag{15}$$

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Once the data is transformed into y_i

- Use a threshold $y_0 \Rightarrow x \in C_1$ iff $y(x) \geq y_0$ or $x \in C_2$ iff $y(x) < y_0$

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Finally

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Once the data is transformed into y_i

- Use a threshold $y_0 \Rightarrow x \in C_1$ iff $y(x) \geq y_0$ or $x \in C_2$ iff $y(x) < y_0$
- Or ML with a Gussian can be used to classify the new transformed data using a Naive Bayes (Central Limit Theorem and $y = \boldsymbol{w}^T \boldsymbol{x}$ sum of random variables).

Please

Your Reading Material, it is about the Multiclass

4.1.6 Fisher's discriminant for multiple classes AT "Pattern Recognition" by Bishop

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- Actually, they are mappings or projections in linear algebra

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Thus, Can we get more powerful mappings?

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Clearly... Yes

- For example, Principal Components or Singular Value Decomposition's

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Also Known as Karhunen-Loeve Transform

Setup

- Consider a data set of observations $\{\boldsymbol{x}_n\}$ with $n = 1, 2, ..., N$ and $\boldsymbol{x_n} \in R^d$.

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Goal

Project data onto space with dimensionality $m < d$ (We assume m is given)

Dimensional Variance

Remember the Variance Sample in $\mathbb{R}$

$$VAR(X) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})^2}{N-1} \tag{16}$$

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You can do the same in the case of two variables X and Y

$$COV(x, y) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})(y_i - \overline{y})}{N-1} \quad (17)$$

Basically

Principal Component Analysis

- Attempts to maximize the variance in certain vectors

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Principal Component Analysis

- Attempts to maximize the variance in certain vectors

Basically Linear Algebra

- Basically discover the basis that describe best the data dispersion in specific directions

Now, Define

Given the data

$$\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N \tag{18}$$

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Center data

$$\boldsymbol{x}_1 - \overline{\boldsymbol{x}}, \boldsymbol{x}_2 - \overline{\boldsymbol{x}}, ..., \boldsymbol{x}_N - \overline{\boldsymbol{x}} \tag{20}$$

Build the Sample Mean

The Covariance Matrix

$$S=\frac{1}{N-1}\sum_{i=1}^{N}\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)^T \tag{21}$$

Build the Sample Mean

The Covariance Matrix

$$S = \frac{1}{N-1} \sum_{i=1}^{N} \left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right) \left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)^T \tag{21}$$

Properties

1. The ijth value of S is equivalent to σ_{ij}^2.
2. The iith value of S is equivalent to σ_{ii}^2.

Outline

Clearly

We need to build a projection

- Remember a square matrix is basically a projection

$$A\boldsymbol{x} = \boldsymbol{x}' \left\{ \text{Projections into the Column Space} \right.$$

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Thus, we want to have the larger dispesrions

- Why not start with a column space of a single dimension == single vector

Using S to Project Data

For this we use a $\boldsymbol{u}_1$ (The single vector!!!)

- with $\boldsymbol{u}_1^T \boldsymbol{u}_1 = 1$, an orthonormal vector

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Question

- What is the Sample Variance of the Projected Data?

Outline

Thus we have

Variance of the projected data

$$\frac{1}{N-1}\sum_{i=1}^{N}\left[\boldsymbol{u}_1\boldsymbol{x}_i - \boldsymbol{u}_1\overline{\boldsymbol{x}}\right] = \boldsymbol{u}_1^T S \boldsymbol{u}_1 \tag{22}$$

Thus we have

Variance of the projected data

$$\frac{1}{N-1}\sum_{i=1}^{N}\left[\boldsymbol{u}_1\boldsymbol{x}_i - \boldsymbol{u}_1\overline{\boldsymbol{x}}\right] = \boldsymbol{u}_1^T S \boldsymbol{u}_1 \quad (22)$$

Use Lagrange Multipliers to Maximize

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 + \lambda_1\left(1 - \boldsymbol{u}_1^T \boldsymbol{u}_1\right) \quad (23)$$

Derive by $\boldsymbol{u}_1$

We get that

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Then

- $\boldsymbol{u}_1$ is an eigenvector of S.

If we left-multiply by $\boldsymbol{u}_1$

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 = \lambda_1 \tag{25}$$

What about the Second Vector $\boldsymbol{u}_2$?

We have the following optimization problem

$$\begin{aligned} \max \ & \boldsymbol{u}_2^T S \boldsymbol{u}_2 \\ \text{s.t. } & \boldsymbol{u}_2^T \boldsymbol{u}_2 = 1 \\ & \boldsymbol{u}_2^T \boldsymbol{u}_1 = 0 \end{aligned}$$

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We can build the Lagrangian function

$$L\left(\boldsymbol{u}_2, \lambda_1', \lambda_2'\right) = \boldsymbol{u}_2^T S \boldsymbol{u}_2 - \lambda_1' \left(\boldsymbol{u}_2^T \boldsymbol{u}_2 - 1\right) - \lambda_2' \left(\boldsymbol{u}_2^T \boldsymbol{u}_1 - 0\right)$$

Explanation

First the constrained maximize

- We want to to maximize $\boldsymbol{u}_2^T S \boldsymbol{u}_2$ (For the second vector)

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Given that the second eigenvector is orthonormal

- We have then $\boldsymbol{u}_2^T \boldsymbol{u}_2 = 1$

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Given that the second eigenvector is orthonormal

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Under orthonormal vectors

- The covariance goes to zero
  $cov\left(\boldsymbol{u}_1, \boldsymbol{u}_2\right) = \boldsymbol{u}_2^T S \boldsymbol{u}_1 = \boldsymbol{u}_2 \lambda_1 \boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1^T \boldsymbol{u}_2 = 0$

Meaning

The PCA's are perpendicular

$$L\left(\boldsymbol{u}_2, \lambda_1', \lambda_2'\right) = \boldsymbol{u}_2^T S \boldsymbol{u}_2 - \lambda_2' \left(\boldsymbol{u}_2^T \boldsymbol{u}_2 - 1\right) - \lambda_1' \left(\boldsymbol{u}_2^T \boldsymbol{u}_1 - 0\right)$$

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The the derivative with respect to $\boldsymbol{u}_2$

$$\frac{\partial L\left(\boldsymbol{u}_2, \lambda_1', \lambda_2'\right)}{\partial \boldsymbol{u}_2} = 2S\boldsymbol{u}_2 - \lambda_2'\boldsymbol{u}_2 - \lambda_1'\boldsymbol{u}_1 = 0$$

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Then, we note the following

$$\boldsymbol{u}_1^T \left[S - \lambda_1' I\right] \boldsymbol{u}_2 - \lambda_1' \boldsymbol{u}_1^T \boldsymbol{u}_1 = 0$$

Then, we have that

We have because of Orthogonality and Othonormalidad

$$
\begin{aligned}
\boldsymbol{u}_1^T \left[S - \lambda_1' I \right] \boldsymbol{u}_2 - \lambda_1' \boldsymbol{u}_1^T \boldsymbol{u}_1 &= \boldsymbol{u}_1^T S \boldsymbol{u}_2 - \boldsymbol{\lambda_1' u}_1^T \boldsymbol{u}_2 - \lambda_1' \\
&= \boldsymbol{u}_1^T S \boldsymbol{u}_2 - \lambda_1'
\end{aligned}
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&= \boldsymbol{u}_1^T S\boldsymbol{u}_2-\lambda_1'
\end{aligned}
$$

We can prove that

$$
\begin{aligned}
\boldsymbol{u}_1^T S\boldsymbol{u}_2 &= \boldsymbol{u}_2^T S\boldsymbol{u}_1 \\
&= \lambda_1\boldsymbol{u}_2^T u_1 \\
&= 0
\end{aligned}
$$

Thus, we have that

Making this to zero, we have the following implication

$$\boldsymbol{u}_1^T S \boldsymbol{u}_2 - \lambda_1' = 0 \longrightarrow \lambda_1' = 0$$

Therefore, we have

Then, for this setup $\lambda'_1 = 0$

$$S\boldsymbol{u}_2 = \lambda'_2 \boldsymbol{u}_2$$

Therefore, we have

Then, for this setup $\lambda'_1 = 0$

$$S\boldsymbol{u}_2 = \lambda'_2 \boldsymbol{u}_2$$

Proving u_2 is the eigenvector of S

- Corresponding to the second largest eigenvalue λ'_2

Thus, we have

Variance will be the maximum when

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 = \lambda_1 \tag{26}$$

is set to the largest eigenvalue. Also know as the First Principal Component

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By Induction

It is possible for M-dimensional space to define M eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2, ..., \boldsymbol{u}_M$ of the data covariance S corresponding to $\lambda_1, \lambda_2, ..., \lambda_M$ that maximize the variance of the projected data.

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Computational Cost of PCA

1. Full eigenvector decomposition $O\left(d^3\right)$
2. Power Method $O\left(Md^2\right)$ "Golub and Van Loan, 1996)"
3. Use the Expectation Maximization Algorithm

Outline

We have the following steps

Determine covariance matrix

$$S = \frac{1}{N-1} \sum_{i=1}^{N} \left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right) \left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)^T \quad (27)$$

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Generate the decomposition

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With

- Eigenvalues in Σ and eigenvectors in the columns of U.

Then

Project samples $\boldsymbol{x}_i$ into subspaces dim$=k$

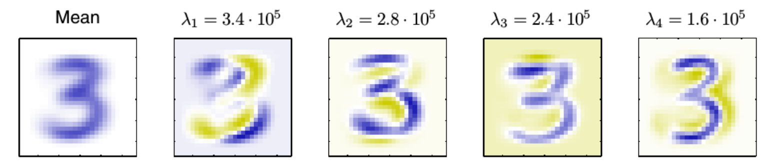
$$z_i = U_K^T \boldsymbol{x}_i$$

- With U_k is a matrix with k columns

Outline

Example

From Bishop



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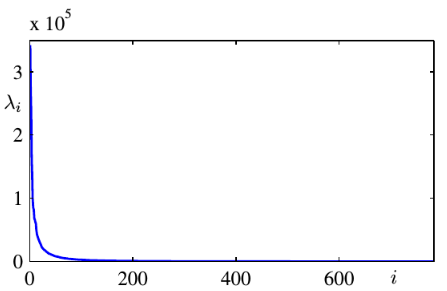

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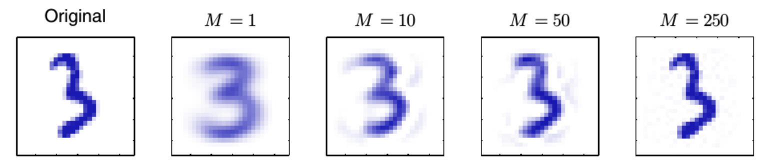

Outline

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We can still diagonalize it

Thus, we can obtain certain properties.

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What happened with no-square matrices

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We want to avoid the problems with

- The decomposition $A = Q\Lambda Q^{-1}$ (Eigendecomposition) because...

The eigenvectors in A have three big problems

1. They are usually not orthogonal.
2. There are not always enough eigenvectors.
3. $A\boldsymbol{x} = \lambda\boldsymbol{x}$ requires A to be square.

Therefore, we can look at the following problem

We have a series of vectors

$$\{\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n\}$$

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Then imagine a set of projection vectors and differences

$$\{\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, ..., \boldsymbol{\alpha}_n\}$$

We want to know a little bit of the relations between them

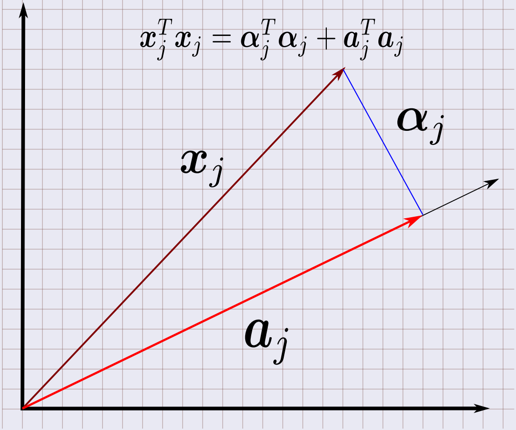
- After all, we are looking at the possibility of using them for our problem

Using the Hypotenuse to build a Relation

A little bit of Geometry, we get

$\boldsymbol{x}_j$	The Data
$\boldsymbol{\alpha}_j$	The Perp defining the projection
$\boldsymbol{a}_j$	The Projection

$$\boldsymbol{x}_j^T\boldsymbol{x}_j = \boldsymbol{\alpha}_j^T\boldsymbol{\alpha}_j + \boldsymbol{a}_j^T\boldsymbol{a}_j$$



Therefore

We have two possible quantities for each j relating them

$$\boldsymbol{\alpha}_j^T \boldsymbol{\alpha}_j = \boldsymbol{x}_j^T \boldsymbol{x}_j - \boldsymbol{a}_j^T \boldsymbol{a}_j$$
$$\boldsymbol{a}_j^T \boldsymbol{a}_j = \boldsymbol{x}_j^T \boldsymbol{x}_j - \boldsymbol{\alpha}_j^T \boldsymbol{\alpha}_j$$

Therefore

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Then, we can minimize and maximize them given that $\boldsymbol{x}_j^T \boldsymbol{x}_j$ is a constant

- Actually, when looking at the previous figure maximize $\boldsymbol{a}_j$ will minimize α_j
  - Which is similar to minimize α_j will maximize $\boldsymbol{a}_j$

Basically

Something Notable when summing over all the sought vectors

$$\min \sum_{j=1}^{n} \boldsymbol{\alpha}_j^T \boldsymbol{\alpha}_j \Leftrightarrow \max \sum_{j=1}^{n} \boldsymbol{a}_j^T \boldsymbol{a}_j$$

Actually this is know as the dual problem (There are many)

An example of this is the following minimization

$$
\begin{aligned}
\min \ \boldsymbol{w}^T\boldsymbol{y}& \\
s.t\ \mathsf{A}\boldsymbol{y} \geq& \boldsymbol{c} \\
\boldsymbol{y} \geq& 0
\end{aligned}
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$$\begin{aligned} \min \ & \boldsymbol{w}^T \boldsymbol{y} \\ s.t \ \mathsf{A}\boldsymbol{y} & \geq \boldsymbol{c} \\ \boldsymbol{y} & \geq 0 \end{aligned}$$

Then, we have the following maximization

$$\begin{aligned} \max \ & \boldsymbol{c}^T \boldsymbol{x} \\ s.t \ \mathsf{A}\boldsymbol{x} & \leq \boldsymbol{c} \\ \boldsymbol{x} & \geq 0 \end{aligned}$$

Outline

We have then

Stack such vectors that in the d-dimensional space the

- In a matrix A of $n \times d$, here each vecrtor has dimension d

$$A = \begin{bmatrix} \boldsymbol{a}_1^T \\ \boldsymbol{a}_2^T \\ \vdots \\ \boldsymbol{a}_n^T \end{bmatrix}$$

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The matrix works as a Projection Matrix

- We are looking for a unit vector $\boldsymbol{v}$ such that length of the projection is maximized.

Why? Do you remember the Projection to a single vector $\boldsymbol{p}$?

Definition of the projection under unitary vector

$$\boldsymbol{p} = \frac{\boldsymbol{v}^T \boldsymbol{a}_i}{\boldsymbol{v}^T \boldsymbol{v}} \boldsymbol{v} = \left[\boldsymbol{v}^T \boldsymbol{a}_i \right] \boldsymbol{v}$$

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Therefore the length of the projected vector is

$$\left\| \left[\boldsymbol{v}^T \boldsymbol{a}_i \right] \boldsymbol{v} \right\| = \left| \boldsymbol{v}^T \boldsymbol{a}_i \right|$$

Then

Thus with a little bit of notation

$$Av = \begin{bmatrix} \boldsymbol{a}_1^T \\ \boldsymbol{a}_2^T \\ \vdots \\ \boldsymbol{a}_n^T \end{bmatrix} \boldsymbol{v} = \begin{bmatrix} \boldsymbol{a}_1^T \boldsymbol{v} \\ \boldsymbol{a}_2^T \boldsymbol{v} \\ \vdots \\ \boldsymbol{a}_n^T \boldsymbol{v} \end{bmatrix}$$

Then

Thus with a little bit of notation

$$A\boldsymbol{v} = \begin{bmatrix} \boldsymbol{a}_1^T \\ \boldsymbol{a}_2^T \\ \vdots \\ \boldsymbol{a}_n^T \end{bmatrix} \boldsymbol{v} = \begin{bmatrix} \boldsymbol{a}_1^T\boldsymbol{v} \\ \boldsymbol{a}_2^T\boldsymbol{v} \\ \vdots \\ \boldsymbol{a}_n^T\boldsymbol{v} \end{bmatrix}$$

Therefore

$$\|A\boldsymbol{v}\| = \sqrt{\sum_{i=1}^{d} \left(\boldsymbol{a}_i^T\boldsymbol{v}\right)^2}$$

Then

It is possible to ask to maximize the longitude of such vector (Singular Vector)

$$\boldsymbol{v}_1 = \arg\max_{\|\boldsymbol{v}\|=1} \|A\boldsymbol{v}\|$$

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Then, we can define the following singular value

$$\sigma_1(A) = \|A\boldsymbol{v}_1\|$$

This is known as

Definition

- The **best-fit line problem** describes the problem of finding the best line for a set of data points, where the quality of the line is measured by the sum of squared (perpendicular) distances of the points to the line.
  - Remember, we are looking at the dual problem....
    - $\min$ sum of squared (perpendicular) distances $\Leftrightarrow$ $\max$ the projections

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    - Remember, we are looking at the dual problem....
        - ★ $\min$ sum of squared (perpendicular) distances $\Leftrightarrow$ $\max$ the projections

Generalization

- This can be transferred to higher dimensions: One can find the best-fit d-dimensional subspace, so the subspace which minimizes the sum of the squared distances of the points to the subspace

Then, in a Greedy Fashion

The second singular vector $\boldsymbol{v}_2$

$$\boldsymbol{v}_2 = \arg \max_{\boldsymbol{v} \perp \boldsymbol{v}_1, \|\boldsymbol{v}\|=1} \|A\boldsymbol{v}\|$$

Then, in a Greedy Fashion

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Them you go through this process

- Stop when we have found all the following vectors:

$$\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r$$

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As singular vectors and

$$\arg \max_{\substack{\boldsymbol{v} \perp \boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r \\ \|\boldsymbol{v}\| = 1}} \|A\boldsymbol{v}\|$$

Proving that the strategy is good

Theorem

- Let A be an $n \times d$ matrix where $\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r$ are the singular vectors defined above. For $1 \leq k \leq r$, let V_k be the subspace spanned by $\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_k$. Then for each k, V_k is the best-fit k-dimensional subspace for A.

Proof

The statement is obviously true for $k = 1$

- What about $k = 2$? Let W be a best-fit 2- dimensional subspace for A.

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For any basis $\boldsymbol{w}_1, \boldsymbol{w}_2$ of W

- $\|A\boldsymbol{w}_1\|^2 + \|A\boldsymbol{w}_2\|^2$ is the sum of the squared lengths of the projections of the rows of A to W.

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For any basis $\boldsymbol{w}_1, \boldsymbol{w}_2$ of W

- $\|A\boldsymbol{w}_1\|^2 + \|A\boldsymbol{w}_2\|^2$ is the sum of the squared lengths of the projections of the rows of A to W.

Now, choose a basis $\boldsymbol{w}_1, \boldsymbol{w}_2$ so that $\boldsymbol{w}_2$ is perpendicular to $\boldsymbol{v}_1$

- This can be a unit vector perpendicular to $\boldsymbol{v}_1$ projection in W.

Do you remember $\boldsymbol{v}_1 = \arg\max_{\|\boldsymbol{v}\|=1} \|A\boldsymbol{v}\|$?

Therefore

$$\|A\boldsymbol{w}_1\|^2 \leq \|A\boldsymbol{v}_1\|^2 \text{ and } \|A\boldsymbol{w}_2\|^2 \leq \|A\boldsymbol{v}_2\|^2$$

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Then

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In a similar way for $k > 2$

- Thus the subspace V_k is at least as good as W and hence is optimal.

Remarks

Every Matrix has a singular value decomposition

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

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Where

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Where

- The columns of U are an orthonormal basis for the column space.
- The columns of V are an orthonormal basis for the row space.
- The Σ is diagonal and the entries on its diagonal $\sigma_i = \Sigma_{ii}$ are positive real numbers, called the singular values of A.

Properties of the Singular Value Decomposition

First

- The eigenvalues of the symmetric matrix $A^T A$ are equal to the square of the singular values of A

$$A^T A = V \Sigma U^T U^T \Sigma V^T = V \Sigma^2 V^T$$

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$$A^T A = V\Sigma U^T U^T \Sigma V^T = V\Sigma^2 V^T$$

Second

- The rank of a matrix is equal to the number of non-zero singular values.

Outline

Singular Value Decomposition as Sums

The singular value decomposition can be viewed as a sum of rank 1 matrices

$$A = A_1 + A_2 + ... + A_R \tag{28}$$

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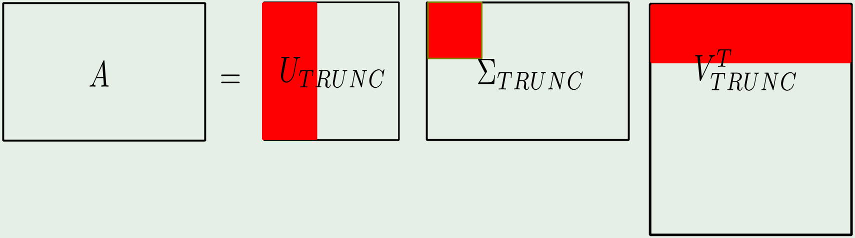
Why?

Decompose $A = U \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_R \end{pmatrix} V^T = \begin{pmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \cdots & \boldsymbol{u}_R \end{pmatrix} \begin{pmatrix} \sigma_1 \boldsymbol{v}_1^T \\ \sigma_2 \boldsymbol{v}_2^T \\ \vdots \\ \sigma_R \boldsymbol{v}_R^T \end{pmatrix}$

$$= \sigma_1 \underbrace{\boldsymbol{u}_1 \boldsymbol{v}_1^T}_{A_1} + \sigma_2 \underbrace{\boldsymbol{u}_2 \boldsymbol{v}_2^T}_{A_2} + \cdots + \sigma_R \underbrace{\boldsymbol{u}_R \boldsymbol{v}_R^T}_{A_R}$$

Truncating

Truncating the singular value decomposition allows us to represent the matrix with less parameters



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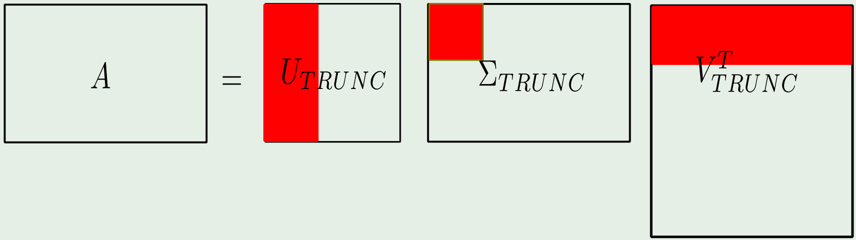

For a 512×512

- Full Representation $512 \times 512 = 262,144$
- Rank 10 approximation $512 \times 10 + 10 + 10 \times 512 = 10,250$

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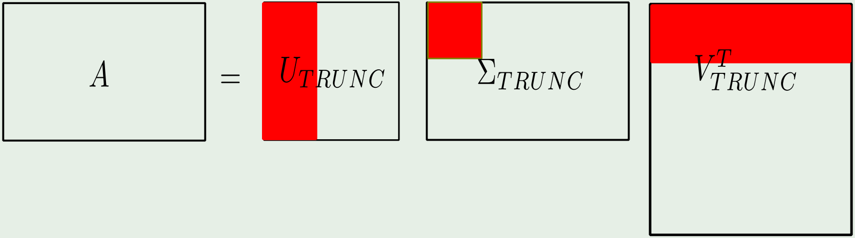

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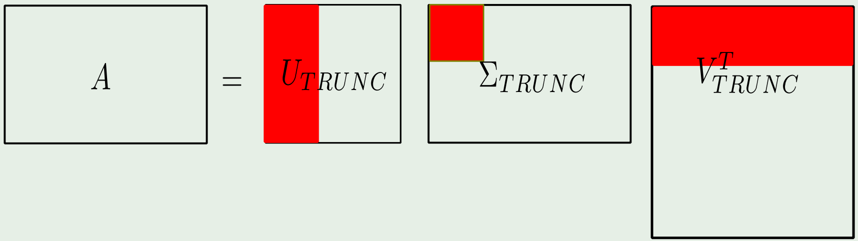

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- Rank 40 approximation $512 \times 40 + 40 + 40 \times 512 = 41,000$
- Rank 80 approximation $512 \times 80 + 80 + 80 \times 512 = 82,000$