Introduction to Machine Learning

Feature Generation

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Outline

1. Fisher Linear Discriminant
   - Introduction
   - The Rotation Idea
   - Solution
     - Scatter measure
   - The Cost Function

2. Principal Components and Singular Value Decomposition
   - Introduction
   - Principal Component Analysis AKA Karhunen-Loeve Transform
     - Projecting the Data
     - Lagrange Multipliers
     - The Process
     - Example
   - Singular Value Decomposition
     - Introduction
     - Building Such Solution
     - Image Compression

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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.

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.

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What Methods we will see?

Fisher Linear Discriminant

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

Principal Component Analysis

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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.

Something Notable

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

Fisher linear discriminant (FLD)

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

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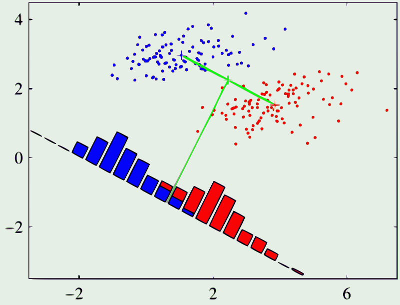
Example

Example - From Left to Right the Improvement



This is actually comming from...

Classifier as

A machine for dimensionality reduction.

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

$$y_i = w^T x_i \quad (1)$$

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Use the mean of each Class

Then

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

We then define the mean sample for ecah class

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

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

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

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

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

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We could simply seek

$$\max \boldsymbol{w}^T \left(\boldsymbol{m}_1 - \boldsymbol{m}_2\right)$$

$$s.t. \sum_{i=1}^{d} w_i = 1$$

After all

We do not care about the magnitude of w.

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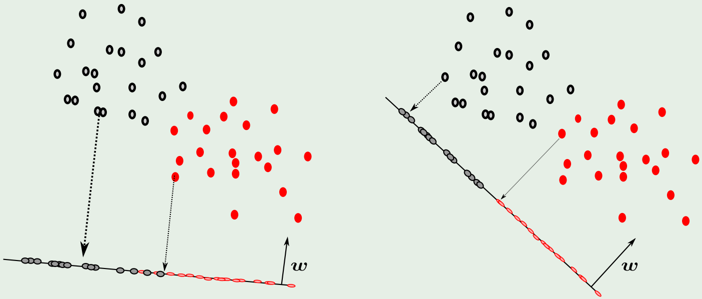
Here, we have the problem



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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.

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

$$s_k^2 = \sum_{x_i \in C_k} \left(w^T x_i - m_k \right)^2 = \sum_{y_i = w^T x_i \in C_k} \left(y_i - m_k \right)^2 \tag{3}$$

We define then within-class variance for the whole data

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

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Finally, a Cost Function

The between-class variance

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

The Fisher criterion

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

Finally

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

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We use a transformation to simplify our life

First

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

Second

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

Third

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

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Now Rename

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^T S_B \boldsymbol{w}}{\boldsymbol{w}^T S_w \boldsymbol{w}} \quad (8)$$

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

Derive with respect to $\boldsymbol{w}$

Thus

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

Then

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

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

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$$\frac{dJ\left(w\right)}{dw} = \frac{S_B}{\left(w^T S_w w\right)} - \frac{w^T S_B w S_w w}{\left(w^T S_w w\right)^2} = 0 \tag{11}$$

Derive with respect to $\boldsymbol{w}$

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Then

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

Derive with respect to $\boldsymbol{w}$

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

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Now, Several Tricks!!!

First

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

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 $\boldsymbol{m}_1 - \boldsymbol{m}_2$!!!

In addition

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

Now, Several Tricks!!!

First

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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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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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1 Fisher Linear Discriminant
- Introduction
- The Rotation Idea
- Solution
  - Scatter measure
- The Cost Function

2 Principal Components and Singular Value Decomposition
- **Introduction**
- Principal Component Analysis AKA Karhunen-Loeve Transform
  - Projecting the Data
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  - Introduction
  - Building Such Solution
  - Image Compression

Did you noticed?

That Rotations really do not exist

- Actually, they are mappings or projections in linear algebra

Thus, Can we get more powerful mappings?

- To obtain better features

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 $\boldsymbol{x_n} \in R^d$.

Goal

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

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Dimensional Variance

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

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

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Given the data

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

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Construct the sample mean

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Center data

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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.

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Using S to Project Data

For this we use a $\boldsymbol{u}_1$

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Question

- What is the Sample Variance of the Projected Data?

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Thus we have

Variance of the projected data

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

Use Lagrange Multipliers to Maximize

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

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Derive by $\boldsymbol{u}_1$

We get

$$S\boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1 \tag{24}$$

Then

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

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

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

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What about the second eigenvector $\boldsymbol{u}_2$

We have the following optimization problem

$$
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Lagrangian

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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)
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Explanation

First the constrained minimization

- We want to to maximize $\boldsymbol{u}_2^T S \boldsymbol{u}_2$

Given that the second eigenvector is orthonormal

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

Under orthonormal vectors

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

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The PCA's are perpendicular

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Thus

Variance will be the maximum when

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 = \lambda_1 \quad (26)$$

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

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.

Computational Cost of PCA

1. Full eigenvector decomposition $O\left(d^3\right)$
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With

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

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- 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

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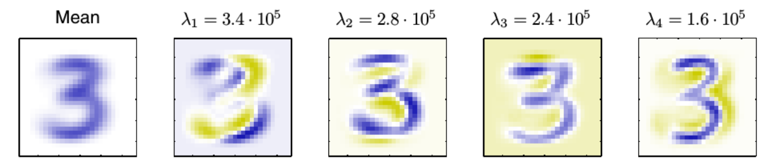
Example

From Bishop



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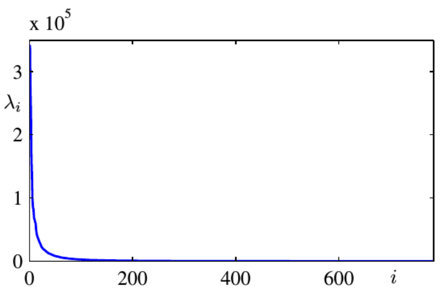

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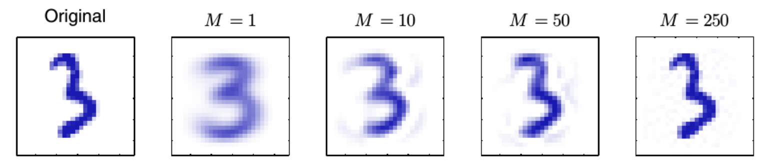

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What happened with no-square matrices

We can still diagonalize it

Thus, we can obtain certain properties.

We want to avoid the problems with

$$S^{-1}AS$$

The eigenvectors in S have three big problems

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Therefore, we can look at the following problem

We have a series of vectors

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Then imagine a set of projection vectors and differences

$$\{\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, ..., \boldsymbol{\beta}_d\} \text{ and } \{\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, ..., \boldsymbol{\alpha}_d\}$$

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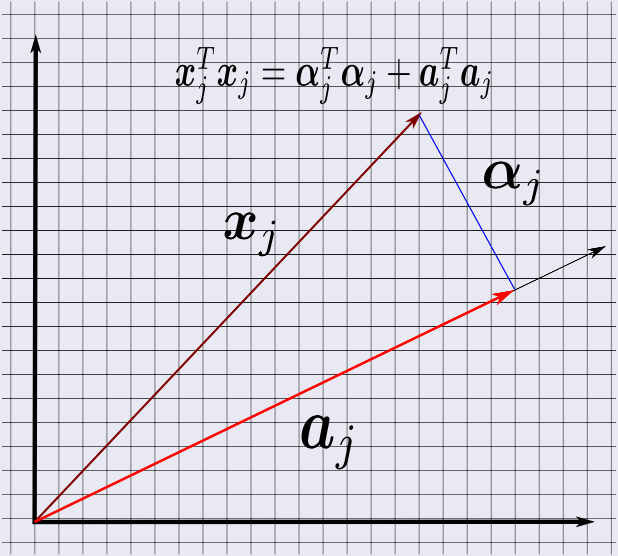
Using the Hypotenuse

A little bit of Geometry, we get



Therefore

We have two possible quantities for each j

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

Then, we can minimize and maximize given that $x_j^T x_j$ is a constant

$$\min \sum_{j=1}^{n} \alpha_j^T \alpha_j$$
$$\max \sum_{j=1}^{n} a_j^T a_j$$

Therefore

We have two possible quantities for each j

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

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

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

Actually this is know as the dual problem (Weak Duality)

An example of this

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

Then, using what is know as slack variables

$$Ax + A'x = b$$

Each row lives in the column space, but the y_i lives in the column space

$$(Ax + A'x)_i \to y_i \text{ and } x' \geq 0$$

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Example of such Slack Matrix

$$(A\boldsymbol{x} + A'\boldsymbol{x}) = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \boldsymbol{x} + \begin{bmatrix} 0 & 0 \\ 0 & -1 \\ -1 & 0 \end{bmatrix} \boldsymbol{x}' = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Element in the column space of dimensionality have three dimensions

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Stack such vectors that in the d-dimensional space the

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

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

Definition of the projection under unitary vector

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

Therefore the length of the projected vector is

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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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- 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.
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Then, in a Greedy Fashion

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

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Them you go through this process

- Stop when we have found all the following vectors:

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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

For $k = 1$

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

For any basis w_1, w_2 of W

- $|Aw_1|^2 + |Aw_2|^2$ is the sum of the squared lengths of the projections of the rows of A to W.

Now, choose a basis w_1, w_2 so that w_2 is perpendicular to v_1

- This can be a unit vector perpendicular to v_1 projection in W.

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In a similar way for $k > 2$

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

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Every Matrix has a singular value decomposition

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

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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

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

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Singular Value Decomposition as Sums

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

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

Why?

$$u_1 A = U \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_R \end{pmatrix} V^T = \begin{pmatrix} u_1 & u_2 & \cdots & u_R \end{pmatrix} \begin{pmatrix} \sigma_1 v_1^T \\ \sigma_2 v_2^T \\ \vdots \\ \sigma_R v_R^T \end{pmatrix}$$

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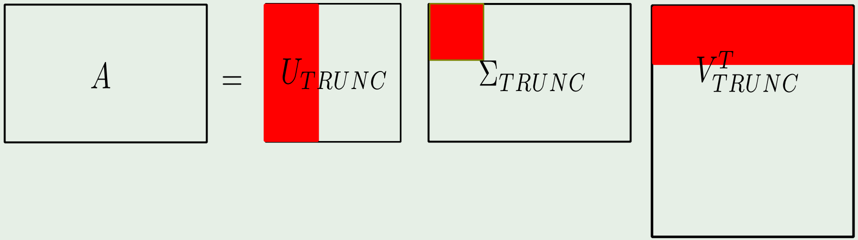
Truncating

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



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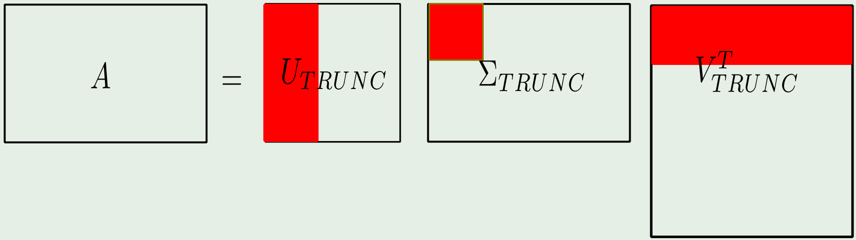

For a 512×512

- Full Representation $512 \times 512 = 262,144$
- Rank 10 approximation $512 \times 10 + 10 + 10 \times 512 = 10,250$
- Rank 40 approximation $512 \times 40 + 40 + 40 \times 512 = 41,000$
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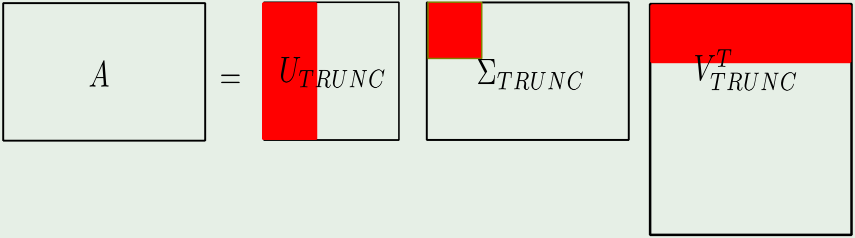

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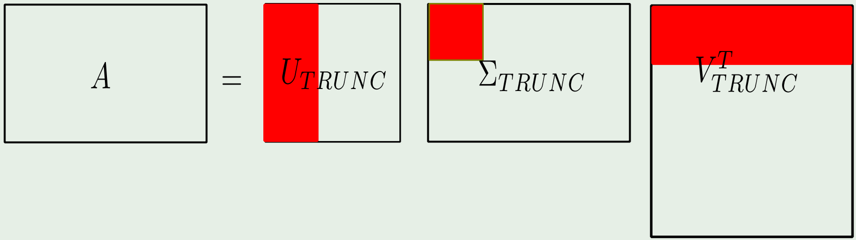

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