Introduction to Machine Learning

Feature Selection and Generation

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Outline

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Why Feature Engineering?

As always we love simple linear models

- Easy to analyze
- Unique solution

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Definition

- Feature engineering (or feature extraction) is the process of using domain knowledge to extract features (characteristics, properties, attributes) from raw data.

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What is this?

Main Question

"Given a number of features, how can one select the most important of them so as to reduce their number and at the same time retain as much as possible of their class discriminatory information? "

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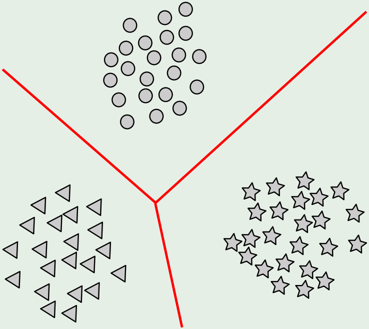
We want features that lead to

1. Large between-class distance.
2. Small within-class variance.

Then

Basically, we want nice separated and dense clusters!!!



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However, Before That...

It is necessary to do the following

1. Outlier removal.

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Actually

PREPROCESSING!!!

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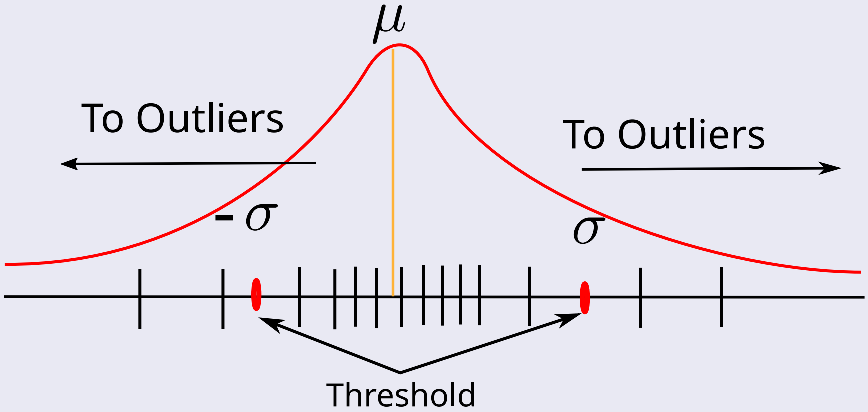
Note

Points with values very different from the mean value produce large errors during training and may have disastrous effects. These effects are even worse when the outliers, and they are the result of noisy measureme

For example, we can use the standard deviation

For a set of samples $x_1, x_2, x_3, \ldots \in \mathbb{R}$



Outlier Removal

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3. For more techniques
   1. Huber, P.J. "Robust Statistics," JohnWiley and Sons, 2nd Ed 2009.

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We can do the following

Algorithm

Input: An $N \times d$ data set $Data$

Output: Candidate Outliers

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4. Return O.

How?

Get the Sample Mean per feature k

$$\boldsymbol{m}_i = \frac{1}{N}\sum_{k=1}^{N} \boldsymbol{x}_{ki}$$

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$$\boldsymbol{m}_i = \frac{1}{N} \sum_{k=1}^{N} \boldsymbol{x}_{ki}$$

Get the Sample Variance per feature k

$$v_i = \frac{1}{N-1} \sum_{k=1}^{N} \left(\boldsymbol{x}_{ki} - \boldsymbol{m}_i\right) \left(\boldsymbol{x}_{ki} - \boldsymbol{m}_i\right)^T$$

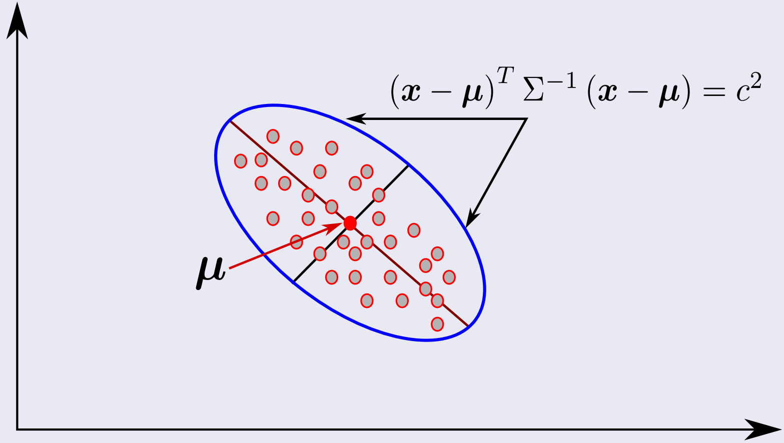
Mahalonobis Distance

We have

$$M\left(\boldsymbol{x}\right) = \sqrt{\left(\boldsymbol{x}-\boldsymbol{\mu}\right)^{T}\Sigma^{-1}\left(\boldsymbol{x}-\boldsymbol{\mu}\right)}$$

Thus

Setting $M(\boldsymbol{x})$ to a constant c defines a multidimensional ellipsoid with centroid at $\boldsymbol{\mu}$



Algorithm

The Partial Code

```
def OutlierRemoval(self, Data):
        SampleMean = Data.mean(1)
        SampleCov  = Data - SampleMean
        SampleCov  = np.cov(SampleCov.T)
        Mahalonobis = (Data - SampleMean)*
                                np.inv(SampleCov)*
                                ((Data - SampleMean).T)

        # Something else here
        # Here you can use chi2.isf(\alpha,dim)
```

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Data Normalization

In the real world

- In many practical situations a designer is confronted with features whose values lie within different dynamic ranges.

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For Example

- We can have two features with the following ranges

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\begin{aligned}
x_i &\in [0, 100, 000] \\
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- Many classification machines will be swamped by the first feature!!!

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Thus!!!

- This does not necessarily reflect their respective significance in the design of the classifier.

Outline

Min-Max Method

Be Naive

- For each feature $i = 1, ..., d$ obtain the $\max_i$ and the $\min_i$ such that

$$\hat{x}_{ik} = \frac{x_{ik} - \min_i}{\max_i - \min_i} \tag{1}$$

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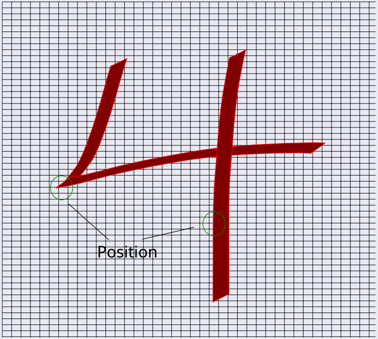
Problem

- This simple normalization will send everything to a unitary sphere!!!
  - However, it works for certain type of data in Deep Learning

However

Even though this can happens there have been report that it can work...

- When data does not depend of single values as:



Gaussian Method

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Everything is Gaussian...

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  1. $\overline{x}_k = \frac{1}{N}\sum_{i=1}^{N} x_{ik},\ k = 1, 2, ..., d$
  2. $\sigma_k^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(x_{ik} - \overline{x}_k\right)^2,\ k = 1, 2, ..., d$

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Thus

$$\hat{x}_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \tag{2}$$

Gaussian Mehtod

Thus

- All new features have zero mean and unit variance.

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However

- We can non-linear mapping. For example the softmax scaling.

Soft Max Scaling

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- It consists of two steps

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First one

$$y_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \tag{3}$$

Soft Max Scaling

Softmax Scaling

- It consists of two steps

First one

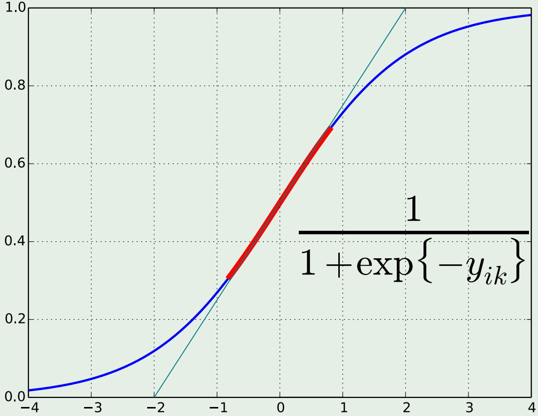
$$y_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \tag{3}$$

Second one

$$\hat{x}_{ik} = \frac{1}{1 + \exp\left\{-y_{ik}\right\}} \tag{4}$$

Explanation

Notice the red area is almost flat!!!



Actually

Thus, we have that

- The red region represents values of y inside of the region defined by the mean and variance (small values of y).
- Then, if we have those values x behaves as a linear function.

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Missing Data

This can happen

In practice, certain features may be missing from some feature vectors.

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Note

Completing the missing values in a set of data is also known as imputation.

Some traditional techniques to solve this problem

Use zeros and risked it!!!

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Does not matter what distribution you have use the sample mean

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Find the distribution of your data

Use the mean from that distribution. For example, if you have a beta distribution

$$\overline{x}_i = \frac{\alpha}{\alpha+\beta} \tag{6}$$

The MOST traditional

Drop it

- Remove that data
  - Still you need to have a lot of data to have this luxury

Outline

Example

We have two matrices

- Data Matrix X
- Missing Data M

$$M_{ij} = \begin{cases} 0 & X_{ij} \text{ is missing} \\ 1 & X_{ij} \text{ is not missing} \end{cases}$$

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This comes from

- "Bayes and multiple imputation" by RJA Little, DB Rubin (2002)

We can use the following optimization

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$$\min_{M_{ij}=1} \|X - AB\|_F$$

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So the total error to be minimized is

$$\min_{M_{ij}=1} \|X - AB\|_F = \sqrt{\sum_{i=1}^{N}\sum_{j=1}^{M}\left[M_{ij}x_{ij} - \sum_{k=1}^{K} a_{ik}b_{kj}\right]^2}$$

- $K \ll N, M$

This can be regularized

Using the following ideas

$$\min_{M_{ij}=1} \|X - AB\|_F + \lambda \left[\|A\|^2 + \|B\|^2 \right]$$

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Therefore, once the minimization is achieved

- We finish with two dense matrices A, B that can be used to obtain the elements with entries $M_{ij} = 0$

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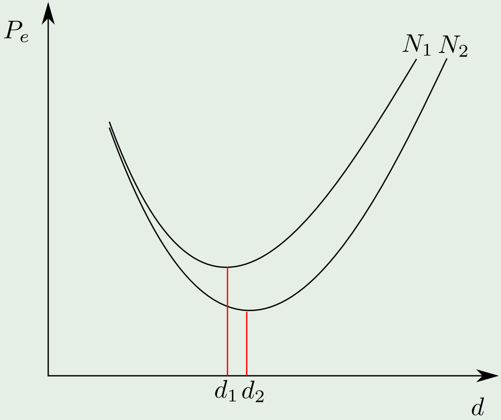
What?

The intuition, the larger the number of samples vs the number of features, the smaller the error P_e

Graphically

For $N_2 \gg N_1$



The Goal of Feature Selection

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- Poor error estimates

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Given N

d must be large enough to learn what makes classes different and what makes patterns in the same class similar

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d must be small enough not to learn what makes patterns of the same class different

In practice

In practice, $d < {}^{N}\!/_{3}$ has been reported to be a sensible choice for a number of cases

Thus

Oh!!!

Once d has been decided, choose the d most informative features:

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Best: Large between class distance, Small within class variance.

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1. Discard individual features with poor information content.

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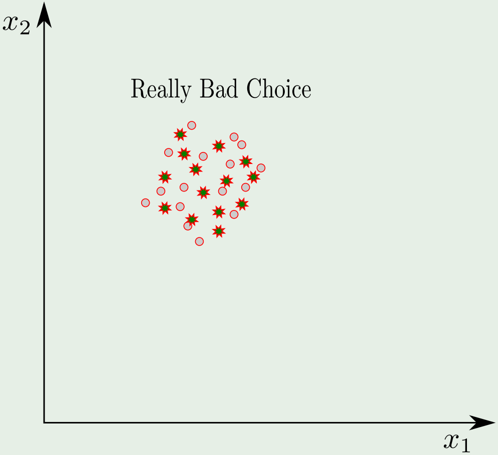
2. The remaining information rich features are examined jointly as vectors

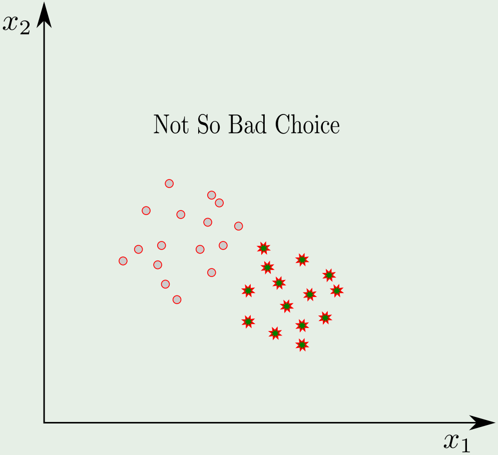
Example

Thus, we want to avoid choices



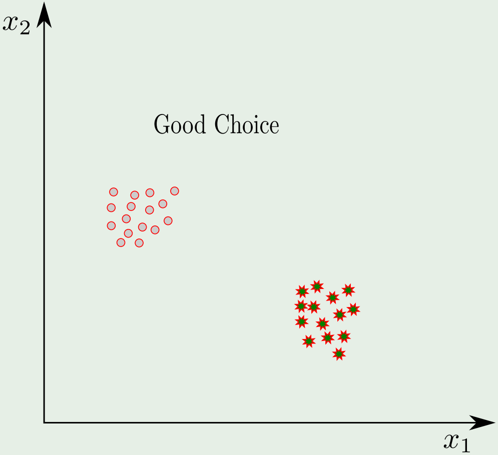
Example

Better Choice



Example

What We Want to Have



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Something Notable

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Then

- Combine features to search for the "best" combination after features have been discarded.

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Possible

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Better

- Adopt a class separability measure and choose the best feature combination against this cost.

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Definition

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$$S_w = \sum_{i=1}^{C} P_i S_i \tag{7}$$

- where C is the number of classes.

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2. P_i the a priori probability of class ω_i defined as $P_i \cong n_i / N$.
   1. n_i is the number of samples in class ω_i.

Scatter Matrices

Between-class scatter matrix

$$S_b = \sum_{i=1}^{C} P_i \left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T \tag{8}$$

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Where

$$\boldsymbol{\mu_0} = \sum_{i=1}^{C} P_i \boldsymbol{\mu}_i \tag{9}$$

The global mean.

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Mixture scatter matrix

$$S_m = E\left[\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T\right] \tag{10}$$

Note: it can be proved that $S_m = S_w + S_b$

Criterion's

First One

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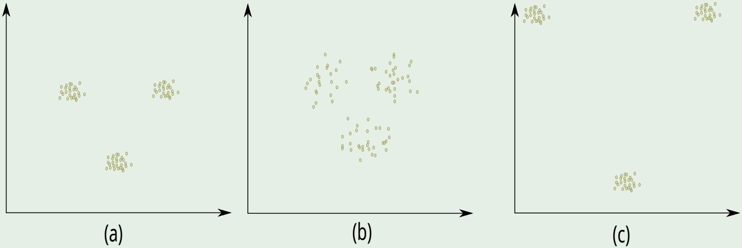
2. $J_3 = trace\left\{S_w^{-1} S_m\right\}$

Example

We have

- Classes with
  - (a) small within-class variance and small between-class distances,
  - (b) large within- class variance and small between-class distances,
  - (c) small within-class variance and large between-class distances.



Outline

What to do with it

We want to avoid

High Complexities

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As for example

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2. Then, get all possible combinations of features

$$\begin{pmatrix} m \\ l \end{pmatrix}$$

with $l = 1, 2, ..., m$

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However these are sub-optimal methods

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Given x_1, x_2, x_3, x_4 and we wish to select two of them

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Adopt a class separability criterion, C, and compute its value for the feature vector $[x_1, x_2, x_3, x_4]^T$.

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Adopt a class separability criterion, C, and compute its value for the feature vector $[x_1, x_2, x_3, x_4]^T$.

Step 2

Eliminate one feature, you get

$$[x_1, x_2, x_3]^T, [x_1, x_2, x_4]^T, [x_1, x_3, x_4]^T, [x_2, x_3, x_4]^T,$$

For example: Sequential Backward Selection

You use your criterion C

Thus the winner is $[x_1, x_2, x_3]^T$

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Now, eliminate a feature and generate $[x_1, x_2]^T, [x_1, x_3]^T, [x_2, x_3]^T$,

Use criterion C

To select the best one

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- The method is sub-optimal
- It suffers of the so called nesting-effect
  - Once a feature is discarded, there is no way to reconsider that feature again.

Similar Problem

For

- Sequential Forward Selection

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For

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We can overcome this by using

- Floating Search Methods

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A more elegant methods are the ones based on

- Dynamic Programming
- Branch and Bound

Outline

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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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.

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

Outline

Did you noticed?

That Rotations really do not exist

- 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

Also Known as Karhunen-Loeve Transform

Setup

- Consider a data set of observations $\{x_n\}$ 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)

Basically

Principal Component Analysis

- Attempts to maximize the variance in certain vectors

Basically

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

$$\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N \tag{12}$$

where $\boldsymbol{x}_i$ is a column vector

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Center data

$$\boldsymbol{x}_1 - \overline{\boldsymbol{x}}, \boldsymbol{x}_2 - \overline{\boldsymbol{x}}, ..., \boldsymbol{x}_N - \overline{\boldsymbol{x}} \tag{14}$$

Build the Sample Mean

The Covariance Matrix

$$S=\frac{1}{N-1}\sum_{i=1}^{N}\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)^T \tag{15}$$

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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

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Thus, we want to have the larger dispersion's

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

Outline

We have the following steps

Determine covariance matrix

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With

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

Then

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

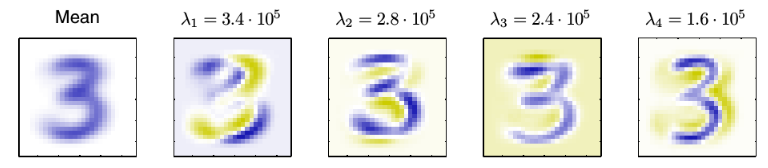
$$z_i = U_K^T \boldsymbol{x}_i$$

- With U_k is a matrix with k columns

Outline

Example

From Bishop



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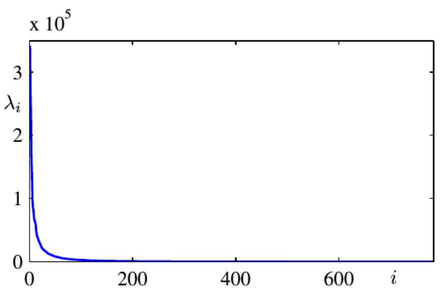

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