The Data Science Cycle

Feature Selection

DataLab

September 21, 2016

Outline

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Outline

Loading Data

We can use Pandas for this!!!

```
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
from scipy.stats import chi2


def ReturnDataFrame(self, path):
        return pd.read_csv(path, sep=',',
                           skipinitialspace=True)

# Load CVS
Path1 = 'SomePath'
DataMatrix = ReturnDataFrame(Path1)

# Transform to an NP Array
Data = DataMatrix.as_matrix()

Data = Data.astype(float)
```

Some properties of the new numpy matrix

We have

$$
\begin{array}{cc}
 & \overbrace{\hphantom{x_{12} \quad \cdots}}^{Features} \\
Samples \left\{ \right. & \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Nd} \end{pmatrix}
\end{array}
$$

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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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2. if information-rich features are selected, the design of the classifier can be greatly simplified.

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

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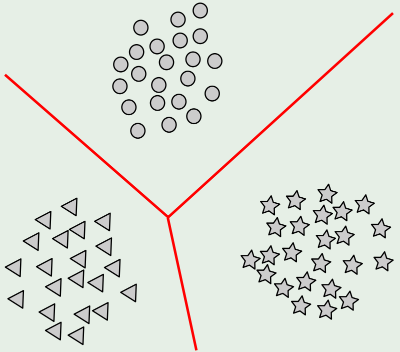
Then

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



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It is necessary to do the following

1. Outliers removal.
2. Data normalization.
3. Deal with missing data.

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For a normally distributed random variable

1. A distance of two times the standard deviation covers 95% of the points.
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Outlier Removal

Important

Then removing outliers is the biggest importance.

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You can do the following

- If you have a small number $\Rightarrow$ discard them!!!

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We can do the following

Algorithm

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

Output: Candidate Outliers

1. Calculate the sample mean μ and sample covariance matrix Σ.
2. Let M be $N \times 1$ vector consisting of square of the Mahalonobis distance to μ.
3. Find points O in M whose values are greater than

$$\chi^2_d(0.05)$$

4. Return O.

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How?

Get the Sample Mean per feature k

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

Get the Sample Variance per feature k

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

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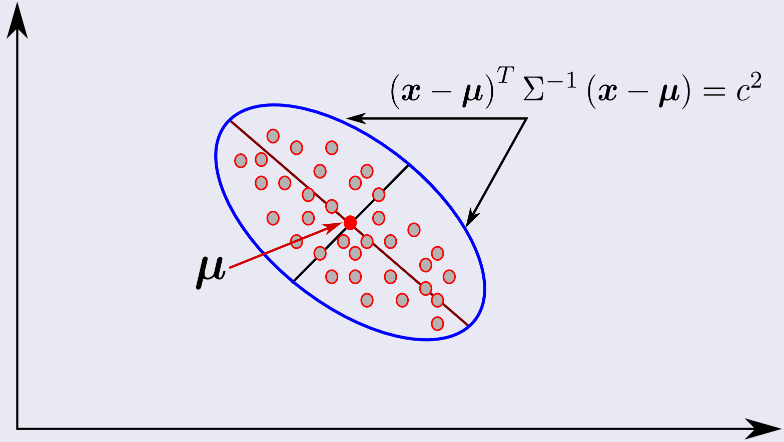
Mahalonobis Distance

We have

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

Why the line 3?

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



As Johnson and Wichern (2007, p. 155, Eq. 4-8) state

The solid ellipsoid of $\boldsymbol{x}$ vectors satisfying

$$(\boldsymbol{x} - \boldsymbol{\mu})^T \, \Sigma^{-1} \, (\boldsymbol{x} - \boldsymbol{\mu}) \leq \chi^2_d \, (\alpha)$$

has a probability $1 - \alpha$.

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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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Outline

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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.

For Example

We can have two features with the following ranges

$$
\begin{aligned}
x_i &\in [0, 100, 000] \\
x_j &\in [0, 0.5]
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Thus

Many classification machines will be swamped by the first feature!!!

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Features with large values may have a larger influence in the cost function than features with small values.

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Naive Normalization

Be Naive

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

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

Problem

This simple normalization will send everything to a unitary sphere thus loosing data resolution!!!

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Gaussian Scaling

Use the idea of

Everything is Gaussian...

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For each feature set...

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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For Example

We have

```python
def GaussianScaling(self, Data):
    SampleMean = np.mean(Data, axis = 0)
    SampleStd  = np.std(Data, axis = 0)

    return (Data-SampleMean)/SampleStd
```

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Missing Data

This can happen

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

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Some traditional techniques to solve this problem

Use zeros and risked it!!!

The idea is not to add anything to the features

The sample mean/unconditional mean

Does not matter what distribution you have use the sample mean

$$\overline{x}_i = \frac{1}{N}\sum_{k=1}^{N} x_{ik} \tag{3}$$

Find the distribution of your data

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

$$\overline{x}_i = \frac{\alpha}{\alpha+\beta} \tag{4}$$

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The MOST traditional

Drop it

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

Outline

THE PEAKING PHENOMENON

Remember

Normally, to design a classifier with good generalization performance, we want the number of sample N to be larger than the number of features d.

What?

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

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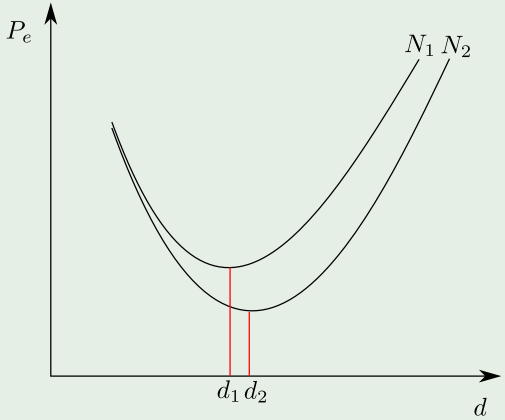
Graphically

For $N_2 \gg N_1$



Let us explain

Something Notable

Let's look at the following example from the paper:

- "A Problem of Dimensionality: A Simple Example" by G.A. Trunk

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Back to Feature Selection

Given N

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

In addition

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

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Oh!!!

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

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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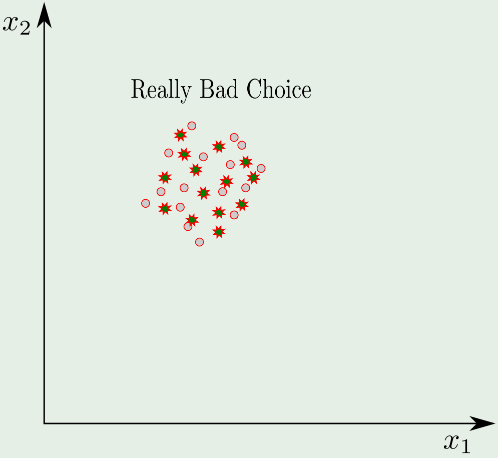
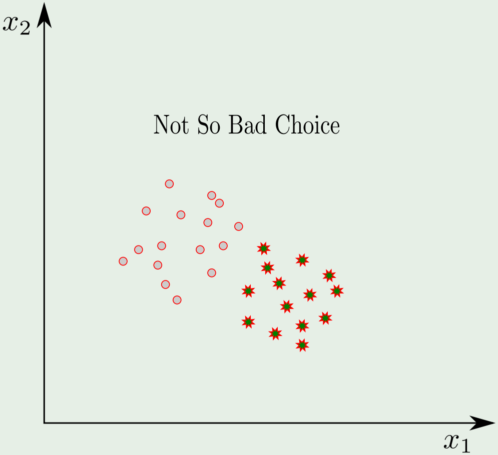
Example

Thus, we want to avoid choices



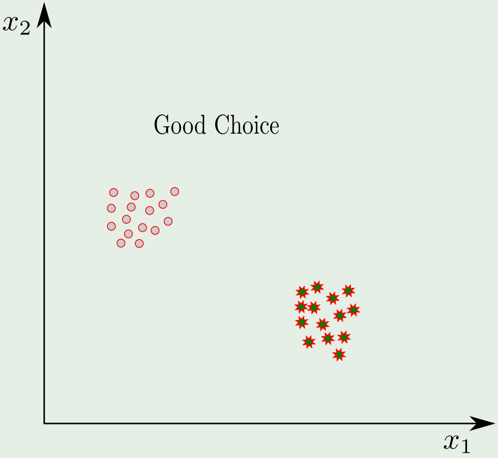
Example

Better Choice



Example

What We Want to Have



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Within-class Scatter Matrix

$$S_w = \sum_{i=1}^{C} P_i \Sigma_i \tag{5}$$

where C is the number of classes.

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Where

We can use the sample mean

$$S_i = E\left[\left(\boldsymbol{x}-\boldsymbol{\mu_i}\right)\left(\boldsymbol{x}-\boldsymbol{\mu_i}\right)^T\right] \approx \frac{1}{N-1}\sum_{k=1}^{n_i}\left(\boldsymbol{x}_{ki}-\boldsymbol{m}_i\right)\left(\boldsymbol{x}_{ki}-\boldsymbol{m}_i\right)^T$$

And P_i the a priori probability of class ω_i defined as

$$P_i \cong n_i/N$$

n_i is the number of samples in class ω_i.

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Scatter Matrices

Between-class scatter matrix

$$S_b = \sum_{i=1}^{C} P_i \left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T \tag{6}$$

Where

$$\boldsymbol{\mu_0} = \sum_{i=1}^{C} P_i \boldsymbol{\mu}_i \tag{7}$$

The global mean.

Mixture scatter matrix

$$S_m = E\left[\left(\boldsymbol{x} - \boldsymbol{\mu}_0\right)\left(\boldsymbol{x} - \boldsymbol{\mu}_0\right)^T\right] \approx \frac{1}{N-1}\sum_{k=1}^{N}\left(\boldsymbol{x}_i - \boldsymbol{\mu}_0\right)\left(\boldsymbol{x}_i - \boldsymbol{\mu}_0\right)^T \tag{8}$$

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

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$$S_m = E\left[\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T\right] \approx \frac{1}{N-1}\sum_{k=1}^{N}\left(\boldsymbol{x}_i - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x}_i - \boldsymbol{\mu_0}\right)^T \tag{8}$$

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

Scatter Matrices

Between-class scatter matrix

$$S_b = \sum_{i=1}^{C} P_i \left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T \tag{6}$$

Where

$$\boldsymbol{\mu_0} = \sum_{i=1}^{C} P_i \boldsymbol{\mu}_i \tag{7}$$

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Criterion

The one we can use

$$J_1 = \frac{trace\left\{S_m\right\}}{trace\left\{S_w\right\}} \tag{9}$$

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Meaning

It takes takes large values when samples in the d-dimensional space are well clustered around their mean, within each class, and the clusters of the different classes are well separated.

Outline

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What to do with it

We want to avoid

High Complexities

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As for example

1. Select a class separability
2. Then, get all possible combinations of features

$$\binom{m}{l}$$

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

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For example: Sequential Backward Selection

We have the following example

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

Step 1

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

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

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You use your criterion C

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

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To select the best one

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Thus, we need

$1 + 1/2((m+1)m - l(l+1))$ combinations

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

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