Introduction to Machine Learning

Feature Selection

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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.

Therefore

We have several attempts for this

- Feature Selection
  - Shrinkage Methods
- Feature Generation
  - Fisher Linear Discriminant
  - Principal Component Analysis
  - Singular Value Decomposition
  - Autoencoders

Basically Feature Engineering

Feature Selection

- Selection of a compact set to avoid the peaking phenomena

Basically Feature Engineering

Feature Selection

- Selection of a compact set to avoid the peaking phenomena

Feature Generation

- Generate Richer Features
  - And select the best ones

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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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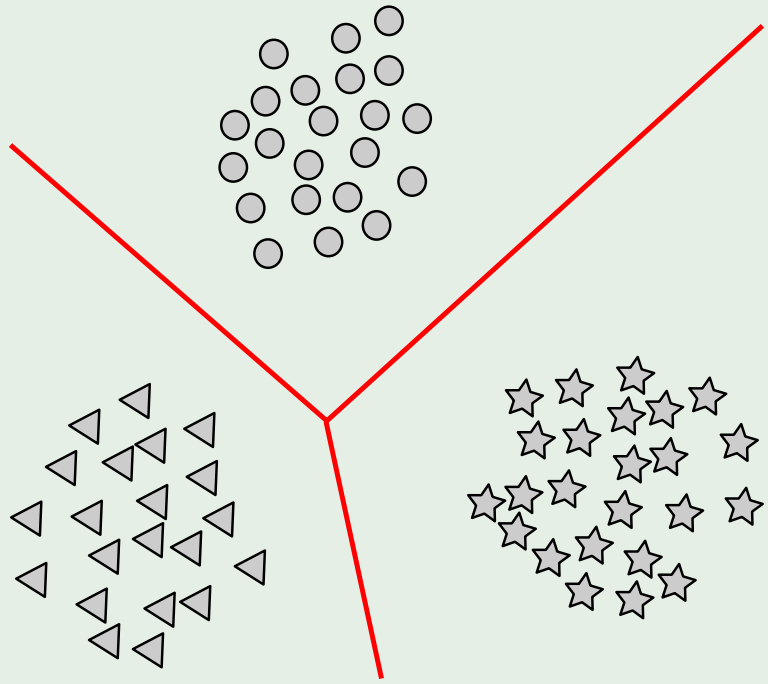
We want features that lead to

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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An outlier is defined as a point that lies very far from the mean of the corresponding random variable.

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2. A distance of three times the standard deviation covers 99% of the points.

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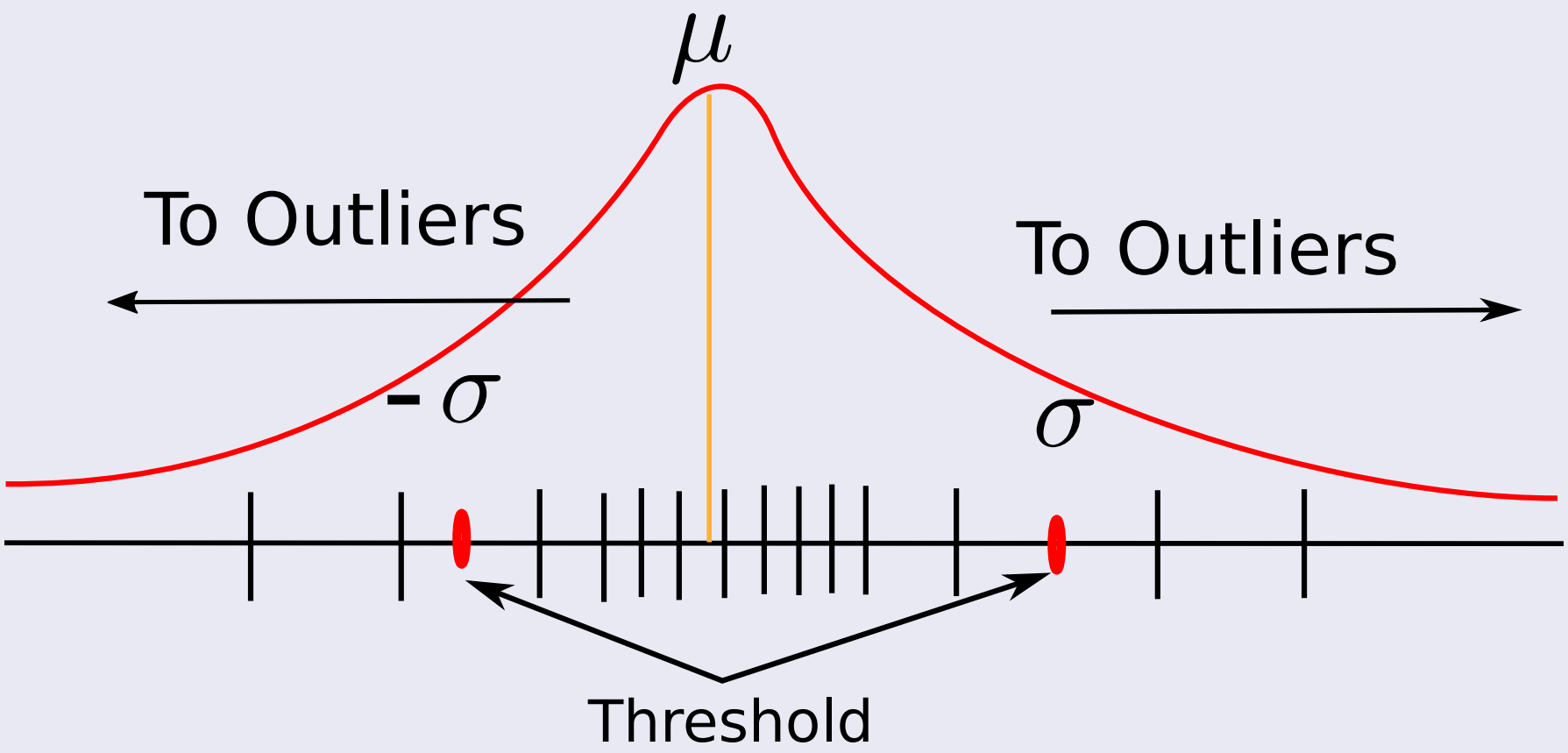
Note

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 $x_1, x_2, x_3, ... \in \mathbb{R}$



Outlier Removal

Important

Then removing outliers is the biggest importance.

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2. Adopt cost functions that are not sensitive to outliers:
3. For more techniques
    1. Huber, P.J. "Robust Statistics," JohnWiley and Sons, 2nd Ed 2009.

An improvement over SD

We can do the following

- Estimate the "middle" of the data, the sample median

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Using order statistics for the samples $x_{(1)} \leq x_{(2)} \leq x_{(3)} \leq ... \leq x_{(n)}$

$$Med(\boldsymbol{x}) = \begin{cases} x_{(m)} & n \text{ is odd for } n = 2m-1 \\ \frac{x_{(m)}+x_{(m+1)}}{2} & n \text{ is even} \end{cases}$$

Then, it is possible

To define a MAD estimator

$$MADN = \frac{Med\{|\boldsymbol{x} - \boldsymbol{Med}(\boldsymbol{x})|\}}{0.6745}$$

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This can be compared with the standard deviation

- The scale constant (approximately 0.6745) is the inverse of the standard normal distribution function evaluated at 3/4.

Something quite interesting

If we use the thresholding to eliminate using SD vs $MADN$

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Why not always use the median and MAD?

- These estimates have statistical poorer performance when outliers do not exist.

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Algorithm

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

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

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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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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

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

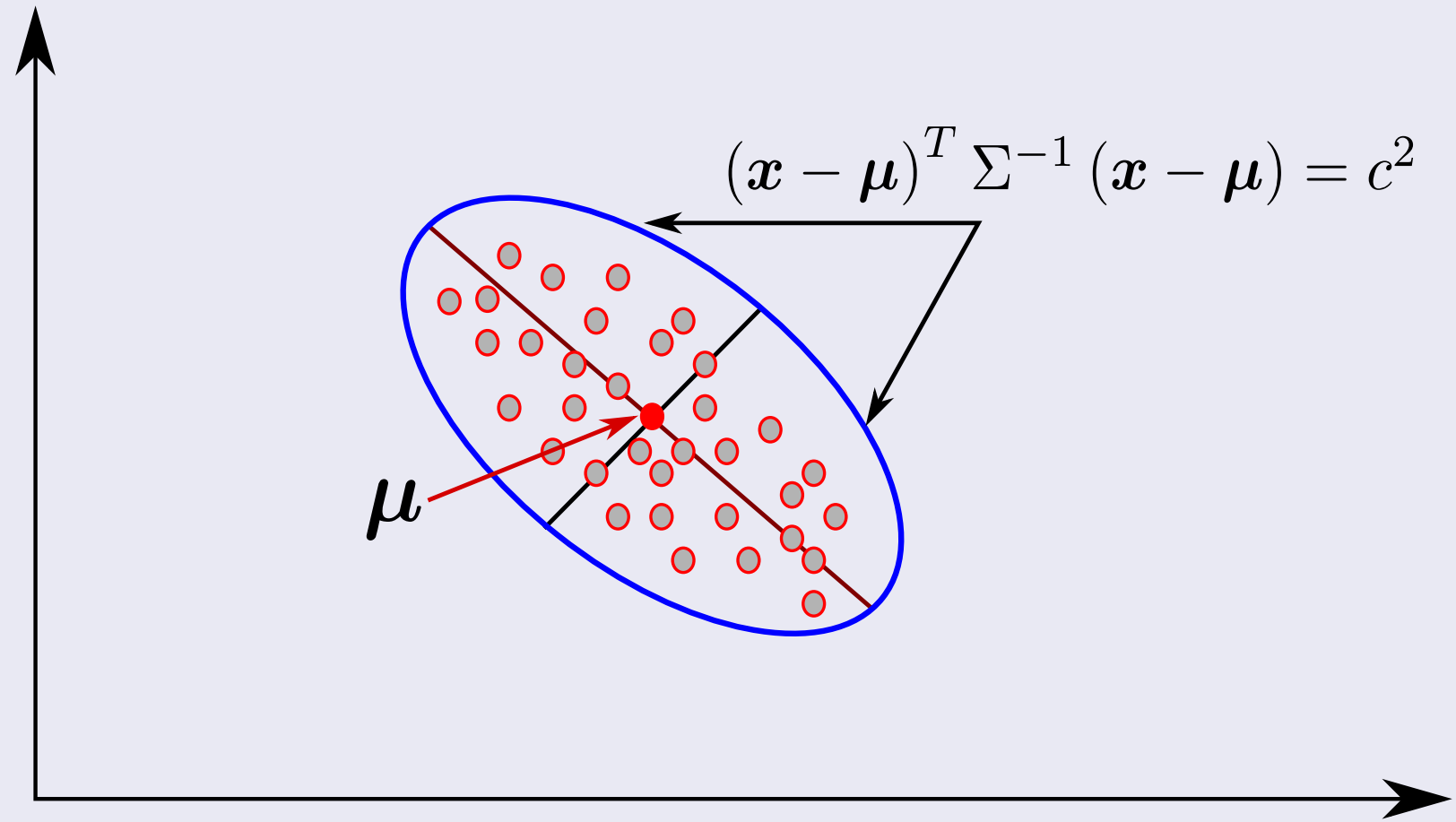
Mahalonobis Distance

We have

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

Thus

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 x vectors satisfying

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

has a probability $1 - \alpha$.

How?

We know that

χ^2_d is defined as the distribution of the sum $\sum_{i=1}^{d} Z_i^2$ where $Z_i's$ are independent $N(0,1)$ random variables.

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Additionally, if we assume that Σ is positive definite and $\Sigma \in \mathbb{R}^{d \times d}$

$$\Sigma = \sum_{i=1}^{d} \lambda_i \boldsymbol{u}_i \boldsymbol{u}_i^T$$

1. $u_i$are the orthonormal eigenvectors of Σ
2. λ_i are the corresponding real eigenvectors

Then

Something Notable

$$\Sigma^{-1} = \sum_{i=1}^{d} \frac{1}{\lambda} \boldsymbol{u}_i \boldsymbol{u}_i^T$$

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Now, if our data matrix element $X \sim N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

We have

$$\Sigma^{-1} \boldsymbol{u}_i = \frac{1}{\lambda_i} \boldsymbol{u}_i$$

Therefore

We have that

$$(X-\boldsymbol{\mu})^T \Sigma^{-1} (X-\boldsymbol{\mu}) = \sum_{i=1}^{d} \frac{1}{\lambda_i} (X-\boldsymbol{\mu})^T \boldsymbol{u}_i \boldsymbol{u}_i^T (X-\boldsymbol{\mu})$$

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Then

$$(X-\boldsymbol{\mu})^T \Sigma^{-1} (X-\boldsymbol{\mu}) = \sum_{i=1}^{d} \left[\frac{1}{\sqrt{\lambda_i}} \boldsymbol{u}_i^T (X-\boldsymbol{\mu}) \right]^2 = \sum_{i=1}^{d} Z_i^2$$

Therefore

If we define

$$\boldsymbol{Z} = \begin{pmatrix} Z_1 \\ Z_2 \\ \vdots \\ Z_d \end{pmatrix}, A_{d\times d} = \begin{pmatrix} \frac{1}{\sqrt{\lambda_1}}\boldsymbol{u}_1^T \\ \frac{1}{\sqrt{\lambda_2}}\boldsymbol{u}_2^T \\ \vdots \\ \frac{1}{\sqrt{\lambda_d}}\boldsymbol{u}_d^T \end{pmatrix}$$

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We know that $(X - \boldsymbol{\mu}) \sim N_d(0, \Sigma)$

- Then, we have $\boldsymbol{Z} = A(X - \boldsymbol{\mu}) \sim N_d\left(0, A\Sigma A^T\right)$

Therefore

Something Notable

$$A\Sigma A^T = \begin{pmatrix} \frac{1}{\sqrt{\lambda_1}}\boldsymbol{u}_1^T \\ \frac{1}{\sqrt{\lambda_2}}\boldsymbol{u}_2^T \\ \vdots \\ \frac{1}{\sqrt{\lambda_d}}\boldsymbol{u}_d^T \end{pmatrix} \left[\sum_{i=1}^{d} \lambda_i \boldsymbol{u}_i \boldsymbol{u}_i^T\right] \begin{pmatrix} \frac{1}{\sqrt{\lambda_1}}\boldsymbol{u}_1 & \frac{1}{\sqrt{\lambda_2}}\boldsymbol{u}_2 & \cdots & \frac{1}{\sqrt{\lambda_d}}\boldsymbol{u}_d \end{pmatrix}$$

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Therefore

$$A\Sigma A^T = \begin{pmatrix} \sqrt{\lambda_1}\boldsymbol{u}_1^T \\ \sqrt{\lambda_2}\boldsymbol{u}_2^T \\ \vdots \\ \sqrt{\lambda_d}\boldsymbol{u}_d^T \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\lambda_1}}\boldsymbol{u}_1 & \frac{1}{\sqrt{\lambda_2}}\boldsymbol{u}_2 & \cdots & \frac{1}{\sqrt{\lambda_d}}\boldsymbol{u}_d \end{pmatrix} = I$$

Therefore

We have that $Z_1, Z_2, ..., Z_d$ are independent standard normal variables

- $(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})$ has a χ^2_d-distribution.

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We have that $Z_1, Z_2, ..., Z_d$ are independent standard normal variables

- $(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})$ has a χ^2_d-distribution.

Finally, the $P\left((\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \leq c^2\right)$

- It is the probability assigned to the ellipsoid $(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \leq c^2$ by the density $N_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Therefore

We have $P\left(\left(\boldsymbol{x}-\boldsymbol{\mu}\right)^{T}\Sigma^{-1}\left(\boldsymbol{x}-\boldsymbol{\mu}\right)\leq\chi_{d}^{2}\left(\alpha\right)\right)=1-\alpha$

Basically $\chi_{d}^{2}\left(\alpha\right)$ is the the critical chi-square value that makes possible the probability $1-\alpha$

Therefore

We have $P\left(\left(\boldsymbol{x}-\boldsymbol{\mu}\right)^{T}\Sigma^{-1}\left(\boldsymbol{x}-\boldsymbol{\mu}\right)\leq\chi_{d}^{2}\left(\alpha\right)\right)=1-\alpha$

Basically $\chi_{d}^{2}\left(\alpha\right)$ is the the critical chi-square value that makes possible the probability $1-\alpha$

Basically

- We assume that if $1-\alpha=.95$ is the data with probability of not being an outlier!!!

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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- We can have two features with the following ranges

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Thus

- 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.

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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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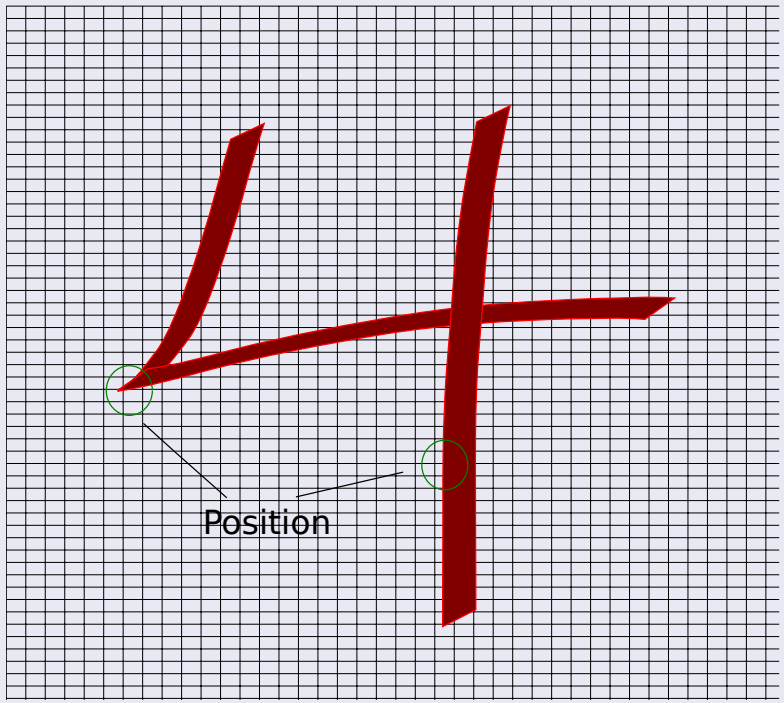
Problem

- 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

Use the idea of

Everything is Gaussian...

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  1. $\overline{x}_k = \frac{1}{N}\sum_{i=1}^{N} x_{ik},\ k = 1, 2, ..., d$

Gaussian Method

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Everything is Gaussian...

Thus

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

Gaussian Method

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Everything is Gaussian...

Thus

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

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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- Other linear techniques limit the feature values in the range of $[0, 1]$ or $[-1, 1]$ by proper scaling.

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

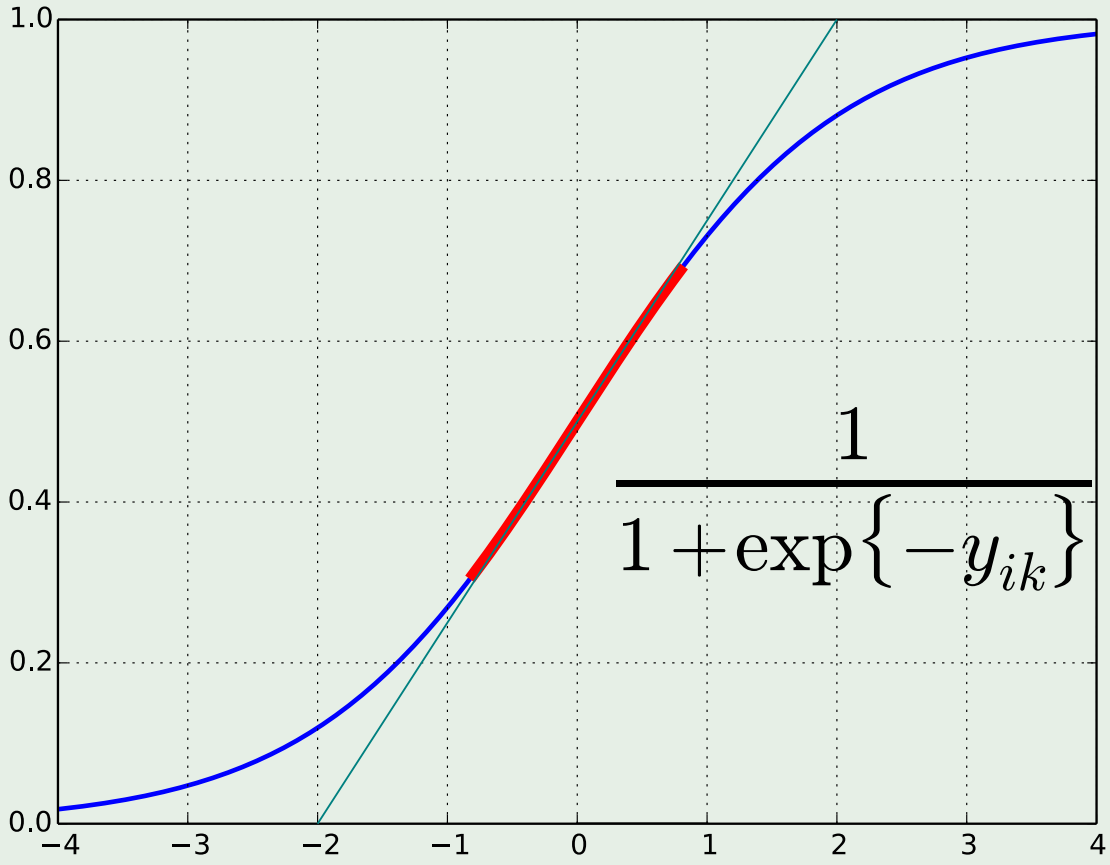
$$y_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \tag{3}$$

Second one

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

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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- 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.

And values too away from the mean

- They are squashed by the exponential part of the function.

If you want a more complex analysis

A more complex analysis

- You can use a Taylor's expansion

$$x = f(y) = f(a) + f'(y)(y-a) + \frac{f''(y)(y-a)^2}{2} + ... \quad (5)$$

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Missing Data

This can happen

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

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Examples where this happens

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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!!!

The idea is not to add anything to the features

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The sample mean/unconditional mean

Does not matter what distribution you have use the sample mean

$$\overline{x}_i = \frac{1}{N}\sum_{k=1}^{N} x_{ik} \tag{6}$$

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Find the distribution of your data

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

$$\overline{x}_i = \frac{\alpha}{\alpha + \beta} \tag{7}$$

The MOST traditional

Drop it

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

Outline

Something more advanced

Split data samples in two set of variables

$$\boldsymbol{x}_{complete} = \begin{pmatrix} \boldsymbol{x}_{observed} \\ \boldsymbol{x}_{missed} \end{pmatrix} \tag{8}$$

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Generate the following probability distribution

$$P\left(\boldsymbol{x}_{missed} | \boldsymbol{x}_{observed}, \Theta\right) = \frac{P\left(\boldsymbol{x}_{missed}, \boldsymbol{x}_{observed} | \Theta\right)}{P\left(\boldsymbol{x}_{observed} | \Theta\right)} \tag{9}$$

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$$P\left(\boldsymbol{x}_{missed} | \boldsymbol{x}_{observed}, \Theta\right) = \frac{P\left(\boldsymbol{x}_{missed}, \boldsymbol{x}_{observed} | \Theta\right)}{P\left(\boldsymbol{x}_{observed} | \Theta\right)} \tag{9}$$

where

$$p\left(\boldsymbol{x}_{observed} | \Theta\right) = \int_{\mathcal{X}} p\left(\boldsymbol{x}_{complete} | \Theta\right) d\boldsymbol{x}_{missed} \tag{10}$$

We can use a Roulette based algorithm

Basically, we use the data to obtain a multivariate version of the data

- Then, we use the α_i in a roulette based algorithm to select a sample
  - Then, we generate $x_{missed} \sim p_j\left(x|\theta\right) + Var\left(x\right)$

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This is the most simple

- What about something more complex?

For this, we can do

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Therefore, we have when integrating the missing (Yes! Marginalization)

$$l_{\boldsymbol{x}_{\boldsymbol{missed}}}\left(\theta\right) = \log \int f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta\right) d\boldsymbol{x}_{\boldsymbol{missed}}$$

Here, it is quite interesting to observe

We have a ratio like this

$$\log \frac{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta\right)}{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta_t\right)}$$

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$$\log \frac{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta\right)}{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta_t\right)}$$

Basically, we can use this function on the EM

$$\begin{aligned} Q\left(\theta|\theta_t\right) =& E_{\theta_t}\left[\log \frac{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta\right)}{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta_t\right)}\right] \\ =& \int \log \frac{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta\right)}{f\left(\boldsymbol{x}_{\boldsymbol{missed}}, \boldsymbol{x}_{\boldsymbol{observed}} | \theta_t\right)} f\left(\boldsymbol{x}_{\boldsymbol{observed}} | \boldsymbol{x}_{\boldsymbol{missed}}, \theta_t\right) d\boldsymbol{x}_{\boldsymbol{observed}} \end{aligned}$$

In this case

Why this ratio?

- Actually, because we want the missing data to be estimated by the observed one

In this case

Why this ratio?

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Actually... There is something quite interesting

- Kullback–Leibler Divergence!!! Yes this ratio is similar

Actually the Kullback–Leibler Divergence

Definition

- For probability distributions P and Q defined on the same probability space, $\mathcal{X}$, the Kullback–Leibler divergence is defined as

$$KL\left(P\left\|Q\right.\right) = \int p\left(x\right) \log\left(\frac{p\left(x\right)}{q\left(x\right)}\right) dx$$

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$$KL(P\|Q) = \int p(x) \log\left(\frac{p(x)}{q(x)}\right) dx$$

Thus, we have that Q is actually a KL version!!!

$$Q(\theta|\theta_t) = \int \log \frac{f(\boldsymbol{x}_{missed}, \boldsymbol{x}_{observed}|\theta)}{f(\boldsymbol{x}_{missed}, \boldsymbol{x}_{observed}|\theta_t)} f(\boldsymbol{x}_{observed}|\boldsymbol{x}_{missed}, \theta_t)\, d\boldsymbol{x}_{observed}$$

$$= \int \log \left(\underbrace{\frac{f(\boldsymbol{x}_{observed}|\boldsymbol{x}_{missed}, \theta) f(\boldsymbol{x}_{missed}|\theta)}{f(\boldsymbol{x}_{observed}|\boldsymbol{x}_{missed}, \theta_t) f(\boldsymbol{x}_{missed}|\theta_t)}}_{\frac{p(x)}{q(x)}} \right) \underbrace{f(\boldsymbol{x}_{obser}|\boldsymbol{x}_{missed}, \theta_t) d\boldsymbol{x}_{obse}}_{p(x)}$$

A Small Problem and Fixing it

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- We have that $\mathcal{L}(\Theta) \geq \mathcal{L}(\Theta_n)$

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So the new Q does not have this difference only the KL

- Basically, the Q lacks a way to enforec this regularization

A simple solution

- As in Ridge Regression

Basically, we can integrate this

Generate a new Q, $l_y(\Theta) - l_y(\Theta_n)$ (EM) and KL Divergence for a Q

$$
\begin{aligned}
Q(\theta|\theta_t) = & \log f(\boldsymbol{x_{missed}}|\theta) \int f(\boldsymbol{x_{observed}}|\boldsymbol{x_{missed}}, \theta_t)\, d\boldsymbol{x_{observed}} - \dots \\
& \log f(\boldsymbol{x_{missed}}|\theta_t) \int f(\boldsymbol{x_{observed}}|\boldsymbol{x_{missed}}, \theta_t)\, d\boldsymbol{x_{observed}} + \dots \\
& \int_{\theta_t} \log \frac{f(\boldsymbol{x_{observed}}|\boldsymbol{x_{missed}}, \theta)}{f(\boldsymbol{x_{observed}}|\boldsymbol{x_{missed}}, \theta_t)} f(\boldsymbol{x_{observed}}|\boldsymbol{x_{missed}}, \theta_t)\, d\boldsymbol{x_{observed}}
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Using a little bit of notation

$$Q(\theta|\theta_t) = l_y(\theta) - l_y(\theta_t) - KL\left(f_{\theta_t}^{\boldsymbol{x_{missed}}} \| f_{\theta}^{\boldsymbol{x_{missed}}}\right)$$

KL-divergence is minimized for $\theta = \theta_t$, actually zero!!!

Then when differentiating the Q divergence

$$\left.\frac{\partial Q\left(\theta|\theta_t\right)}{\partial\theta}\right|_{\theta=\theta_y} = \left.\frac{\partial l_{\boldsymbol{x_{missed}}}\left(\theta\right)}{\partial\theta}\right|_{\theta=\theta_y}$$

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Thus define the iteration as

$$\theta_{t+1} = \arg\max_{\theta} Q\left(\theta|\theta_t\right)$$

It is possible to see that

Something Notable

$$Q\left(\theta_{t+1}|\theta_t\right) + l_y\left(\theta_t\right) + KL\left(f_{\theta_t}^{\boldsymbol{x_{missed}}} \middle\| f_{\theta_t}^{\boldsymbol{x_{missed}}}\right) = l_y\left(\theta_{t+1}\right)$$

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Then

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Thus

- The log-likelihood never decreases after a combined $E - step$ and $M - step$.

Here, everything looks great but...

We need to know to which distribution could come the result

- Thus, we have that we assume that the missing data can come from two distributions!!!

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We need to know to which distribution could come the result

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Start from the simple

- We assume a two possible sources of the information for the missing data.

Thus, we can device the following Likelihood

We can consider a sample $Y = \{Y_1, ..., Y_n\}$ from individual densities

$$f(y|\alpha, \mu) = \alpha\phi(y - \mu) + (1 - \alpha)\phi(y)$$

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$$f(y|\alpha, \mu) = \alpha\phi(y - \mu) + (1 - \alpha)\phi(y)$$

Where, we can impose the following distribution

$$\phi(y) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{y^2}{2}\right\}$$

- With both α and μ are both unknown, but $0 < \alpha < 1$.

Incomplete observation

The likelihood function becomes

$$L_{\boldsymbol{x_{missed}}}(\alpha, \mu) = \prod_{i=1}^{N} \alpha\phi(y_i - \mu) + (1 - \alpha)\phi(y_i)$$

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This is a quite unpleasant function

- But suppose we knew which observations came from which population?

What?

Let $X = \{x_1, ..., x_n\}$ be i.i.d. with $P(x_i = 1) = \alpha$

- Then, we play the hierarchical idea

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Hierachy

$$y_i \sim N(\mu, 1) \text{ if } x_i = 1$$
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Hierachy

$$y_i \sim N(\mu, 1) \text{ if } x_i = 1$$
$$y_i \sim N(0, 1) \text{ if } x_i = 0$$

i.e x_i allows to indicate to which distribution y_i belongs

- Then we need the marginal distribution of Y.

Thus

The Complete Data Likelihood is

$$L_{x,y}(\alpha,\mu)=\prod_{i=1}^{N}\alpha^{x_i}\phi(y_i-\mu)^{x_i}(1-\alpha)^{1-x_i}\phi(y_i)^{1-x_i}$$

Thus

The Complete Data Likelihood is

$$L_{x,y}(\alpha,\mu)=\prod_{i=1}^{N}\alpha^{x_i}\phi(y_i-\mu)^{x_i}(1-\alpha)^{1-x_i}\phi(y_i)^{1-x_i}$$

Or given that $\phi(y_i)$ does not contain any parameter

$$L_{x,y}(\alpha,\mu)\propto\alpha^{\sum x_i}(1-\alpha)^{n-\sum x_i}\prod_{i=1}^{N}\phi(y_i-\mu)^{x_i}$$

Then taking logarithms

We have that

$$l_{x,y}(\alpha,\mu)=\sum x_i\log\alpha+\left(n-\sum x_i\right)\log(1-\alpha)-\sum\frac{x_i\left(y_i-\mu\right)^2}{2}$$

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Therefore, if we differentiate

$$\widehat{\alpha}=\frac{1}{x_i}\sum x_i,\widehat{\mu}=\frac{\sum x_iy_i}{\sum x_i}$$

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We have seen this formulations

- The EM algorithm for the Mixture of Gaussian's

Outline

Example

We have two matrices

- Data Matrix X
- Missing Data M

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

Example

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This comes from

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

We can use the following optimization

We can do the following

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

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$$M_{ij}x_{ij} \approx \sum_{k=1}^{K} a_{ik}b_{kj}$$

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 $M_{ij} = 0$

There are many other methods for this

For example

- Moritz Hardt. Understanding Alternating Minimization for Matrix Completion. FOCS, pages 651–660, 2014.
- Moritz Hardt, Mary Wootters. Fast matrix completion without the condition number. COLT, pages 638–678, 20
- Raghunandan H Keshavan, Andrea Montanari, and Sewoong Oh, Matrix completion from noisy entries, The Journal of Machine Learning Research 99 (2010), 2057–2078.
- Stephen J Wright, Robert D Nowak, and M´ario AT Figueiredo, Sparse reconstruction by separable approximation, Signal Processing, IEEE Transactions on 57 (2009), no. 7, 2479–2493.

Outline

THE PEAKING PHENOMENON

Remeber

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.

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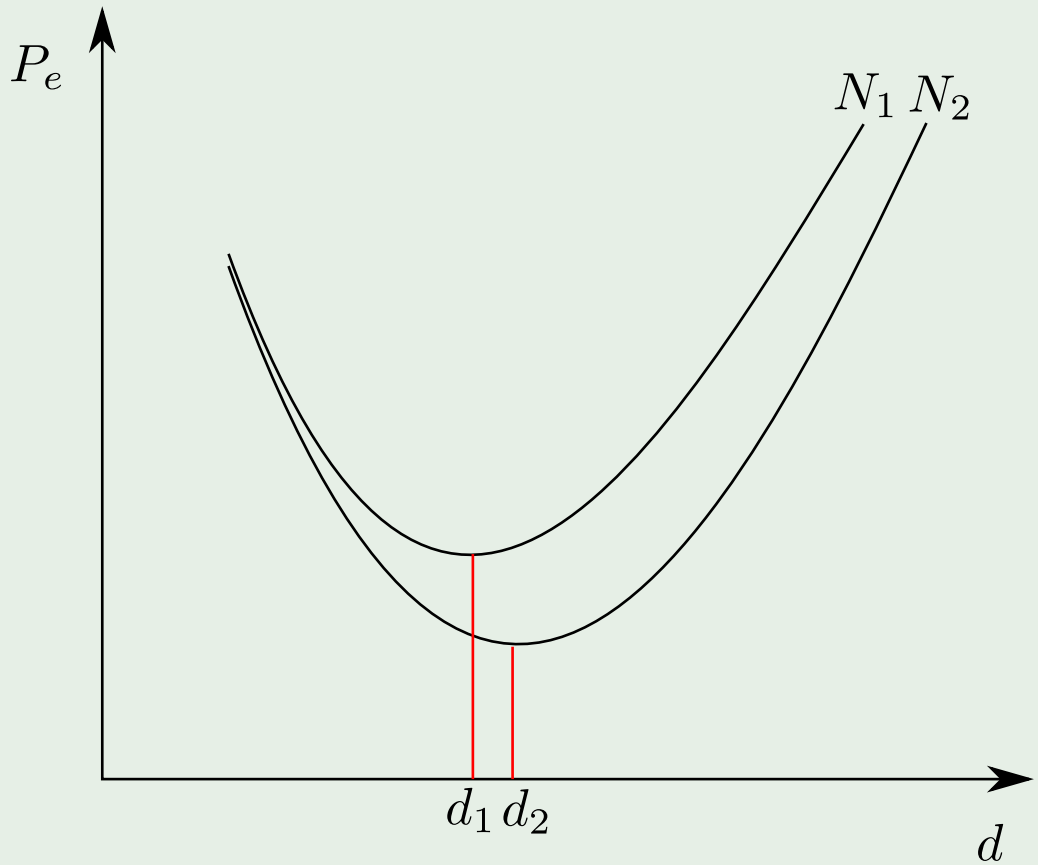
What?

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

Graphically

For $N_2 \gg N_1$



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

THE PEAKING PHENOMENON

Assume the following problem

We have two classes ω_1, ω_2 such that

$$P(\omega_1) = P(\omega_2) = \frac{1}{2} \tag{11}$$

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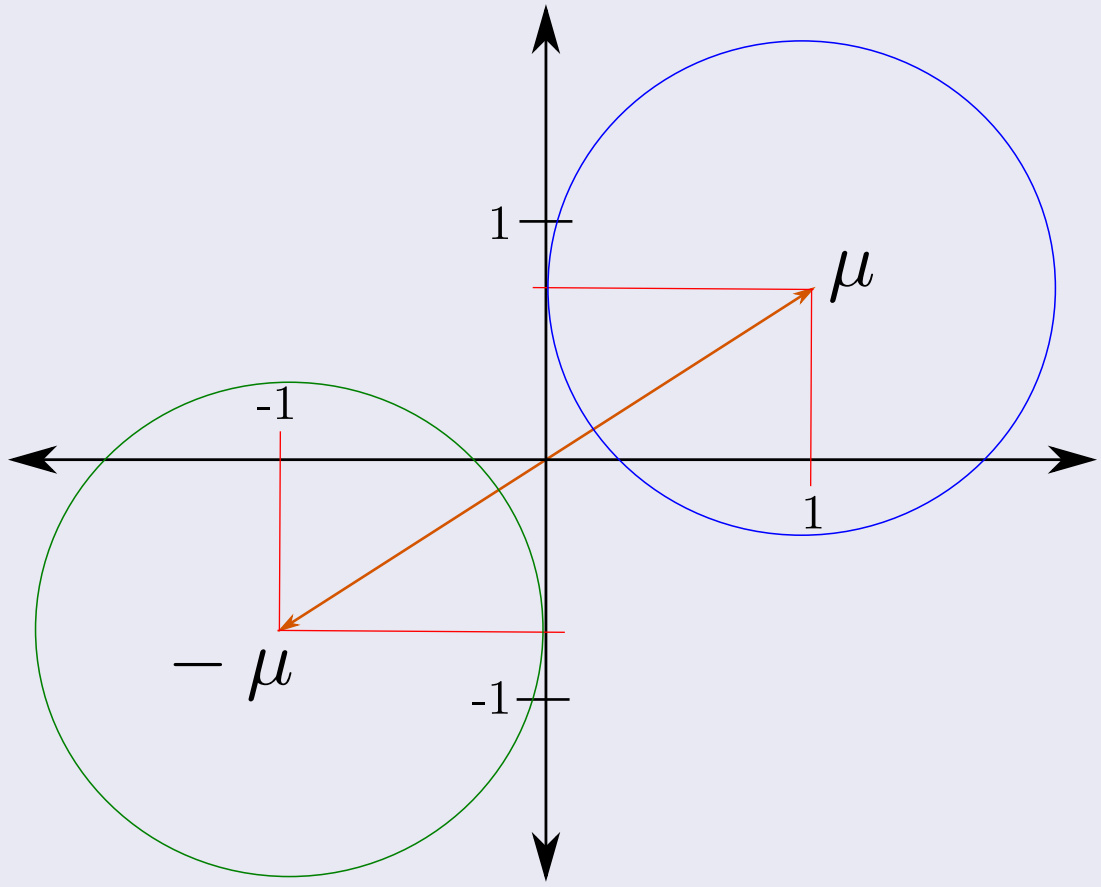
Where

$$\mu = \left[1, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, ..., \frac{1}{\sqrt{d}}\right]$$

Example

The μ for $\mathbb{R}^2$

$$\mu = \left(1, \frac{1}{\sqrt{2}}\right)^T$$



THE PEAKING PHENOMENON

Properties of the features

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2. $z \equiv \boldsymbol{x}^T \boldsymbol{\mu} < 0$ then $\boldsymbol{x} \in \omega_2$.

A little bit of algebra

For the first case

$$(\boldsymbol{x}-\boldsymbol{\mu})^T(\boldsymbol{x}-\boldsymbol{\mu}) < (\boldsymbol{x}+\boldsymbol{\mu})^T(\boldsymbol{x}+\boldsymbol{\mu})$$
$$\boldsymbol{x}^t\boldsymbol{x} - \boldsymbol{2x^T\mu} + \boldsymbol{\mu^T\mu} < \boldsymbol{x}^t\boldsymbol{x} + \boldsymbol{2x^T\mu} + \boldsymbol{\mu^T\mu}$$
$$0 < \boldsymbol{x^T\mu} \equiv z$$

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For the first case

$$\boldsymbol{x^t x - 2x^T \mu + \mu^T \mu < x^t x + 2x^T \mu + \mu^T \mu}$$

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We have then two cases

1. Known mean value μ.
2. Unknown mean value μ.

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$$\begin{aligned}\|\boldsymbol{x}-\boldsymbol{\mu}\|^2 &< \|\boldsymbol{x}+\boldsymbol{\mu}\|^2 \\ (\boldsymbol{x}-\boldsymbol{\mu})^T(\boldsymbol{x}-\boldsymbol{\mu}) &< (\boldsymbol{x}+\boldsymbol{\mu})^T(\boldsymbol{x}+\boldsymbol{\mu}) \\ \boldsymbol{x}^t\boldsymbol{x}-\boldsymbol{2x^T\mu}+\boldsymbol{\mu^T\mu} &< \boldsymbol{x}^t\boldsymbol{x}+\boldsymbol{2x^T\mu}+\boldsymbol{\mu^T\mu} \\ 0 &< \boldsymbol{x^T\mu} \equiv z\end{aligned}$$

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Given that z is a linear combination of independent Gaussian Variables

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2. $E[z] = \sum_{i=1}^{d} \mu_i E(x_i) = \sum_{i=1}^{d} \frac{1}{\sqrt{i}} \frac{1}{\sqrt{i}} = \sum_{i=1}^{d} \frac{1}{i} = \|\boldsymbol{\mu}\|^2$.

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It can be seen as random variable with mean $\frac{1}{\sqrt{i}}$ and variance 1 with no correlation between each other.

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What about the variance of z?

$$
\begin{aligned}
&= E\left[z^2 - 2z\left\|\boldsymbol{\mu}\right\|^2 + \left\|\boldsymbol{\mu}\right\|^4\right] \\
&= E\left[\boldsymbol{z}^2\right] - \left\|\boldsymbol{\mu}\right\|^4 \\
&= E\left[\left(\sum_{i=1}^{d} \mu_i x_i\right)\left(\sum_{i=1}^{d} \mu_i x_i\right)\right] - \left(\sum_{i=1}^{d} \frac{1}{i^2} + \sum_{\substack{j=1 \\ j \neq h}}^{d} \sum_{h=1}^{d} \frac{1}{i} \times \frac{1}{j}\right)
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$$= E\left[\boldsymbol{z}^2\right] - \|\boldsymbol{\mu}\|^4$$

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What about the variance of z?

$$
\begin{aligned}
Var\left(\boldsymbol{z}\right) =& E\left[\left(z - \left\|\boldsymbol{\mu}\right\|^2\right)^2\right] \\
=& E\left[z^2 - 2z\left\|\boldsymbol{\mu}\right\|^2 + \left\|\boldsymbol{\mu}\right\|^4\right] \\
=& E\left[\boldsymbol{z}^2\right] - \left\|\boldsymbol{\mu}\right\|^4 \\
=& E\left[\left(\sum_{i=1}^{d} \mu_i x_i\right)\left(\sum_{i=1}^{d} \mu_i x_i\right)\right] - \left(\sum_{i=1}^{d} \frac{1}{i^2} + \sum_{\substack{j=1 \\ j\neq h}}^{d}\sum_{h=1}^{d} \frac{1}{i} \times \frac{1}{j}\right)
\end{aligned}
$$

Thus

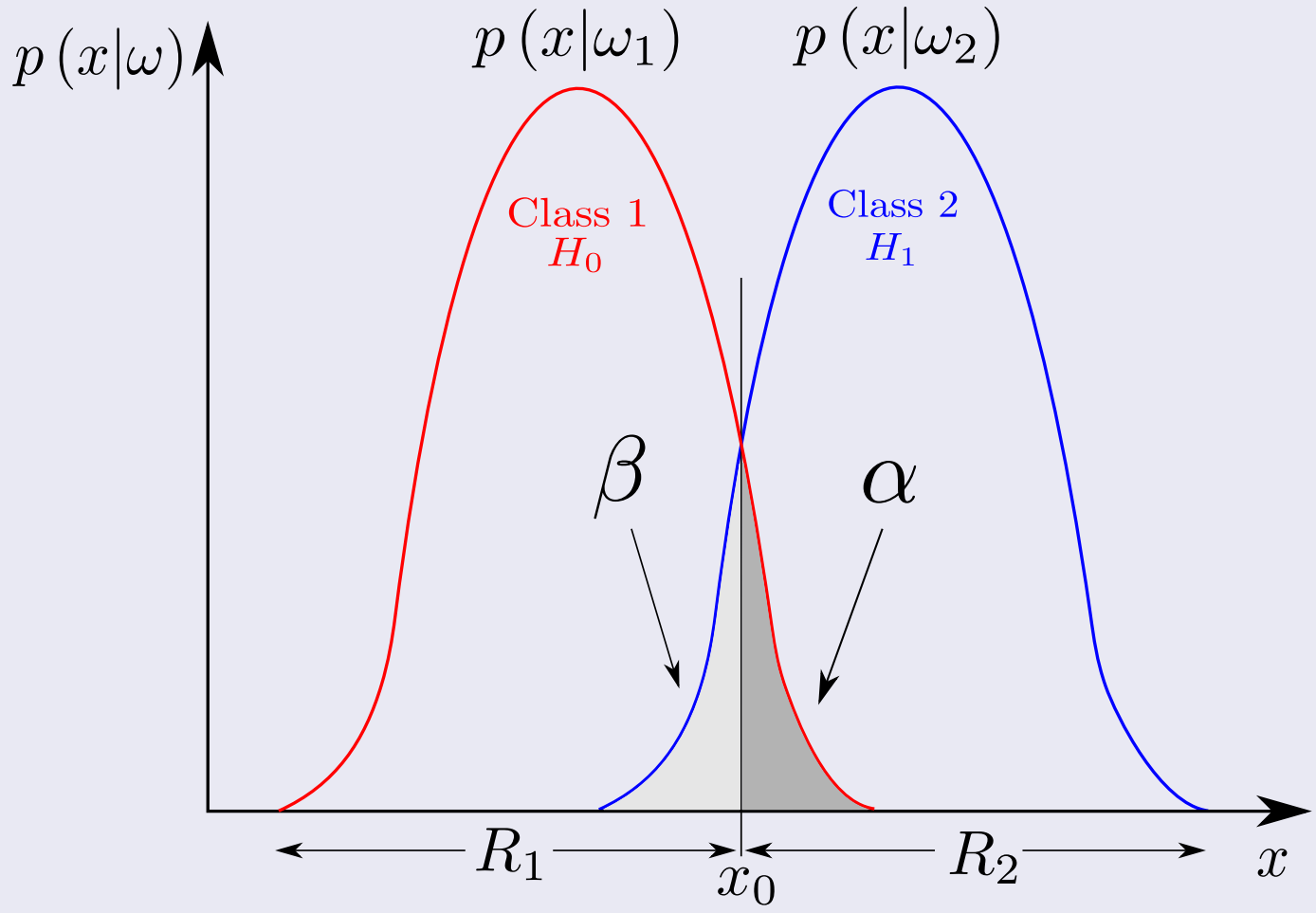
But, given that $x_i^2 \sim \chi_1^2\left(\frac{1}{i}\right)$, with mean

$$E\left[x_i^2\right] = 1 + \frac{1}{i} \tag{12}$$

Remark: The rest is for you to solve so $\sigma_z^2 = \|\boldsymbol{\mu}\|^2$.

Remember the P_e

We have then...



We get the probability of error

We know that the error is coming from the following equation

$$P_e = \frac{1}{2}\int_{-\infty}^{x_0} p\left(z|\omega_2\right) d\boldsymbol{x} + \frac{1}{2}\int_{x_0}^{\infty} p\left(z|\omega_1\right) d\boldsymbol{x} \tag{13}$$

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Thus, we have that

Now, given that z is a sum of Gaussian

$$\text{exp term} = -\frac{1}{2\left\|\boldsymbol{\mu}\right\|^2}\left[\left(z-\left\|\boldsymbol{\mu}\right\|^2\right)^2\right] \tag{14}$$

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Because we have the rule

We can do a change of variable to a normalized z

$$P_e = \int_{b_d}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{z^2}{2}\right\} dz \tag{15}$$

Known mean value μ

The probability of error is given by

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Where

$$b_d = \sqrt{\sum_{i=1}^{d} \frac{1}{i}} \tag{17}$$

How?

Known mean value μ

Thus

When the series b_d tends to infinity as $d \to \infty$, the probability of error tends to **zero** as the number of features increases.

Unknown mean value μ

For This, we use the maximum likelihood

$$\widehat{\boldsymbol{\mu}} = \frac{1}{N}\sum_{k=1}^{N} s_k \boldsymbol{x}_k \tag{18}$$

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$$b_d = \frac{E[z]}{\sigma_z} \tag{19}$$

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Thus, using P_e

- It can now be shown that $b_d \to 0$ as $d \to \infty$ and the probability of error tends to $\frac{1}{2}$ for any finite number N.

Finally

Case I

- If for any d the corresponding PDF is known, then we can perfectly discriminate the two classes by arbitrarily increasing the number of features.

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Case I

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Case II

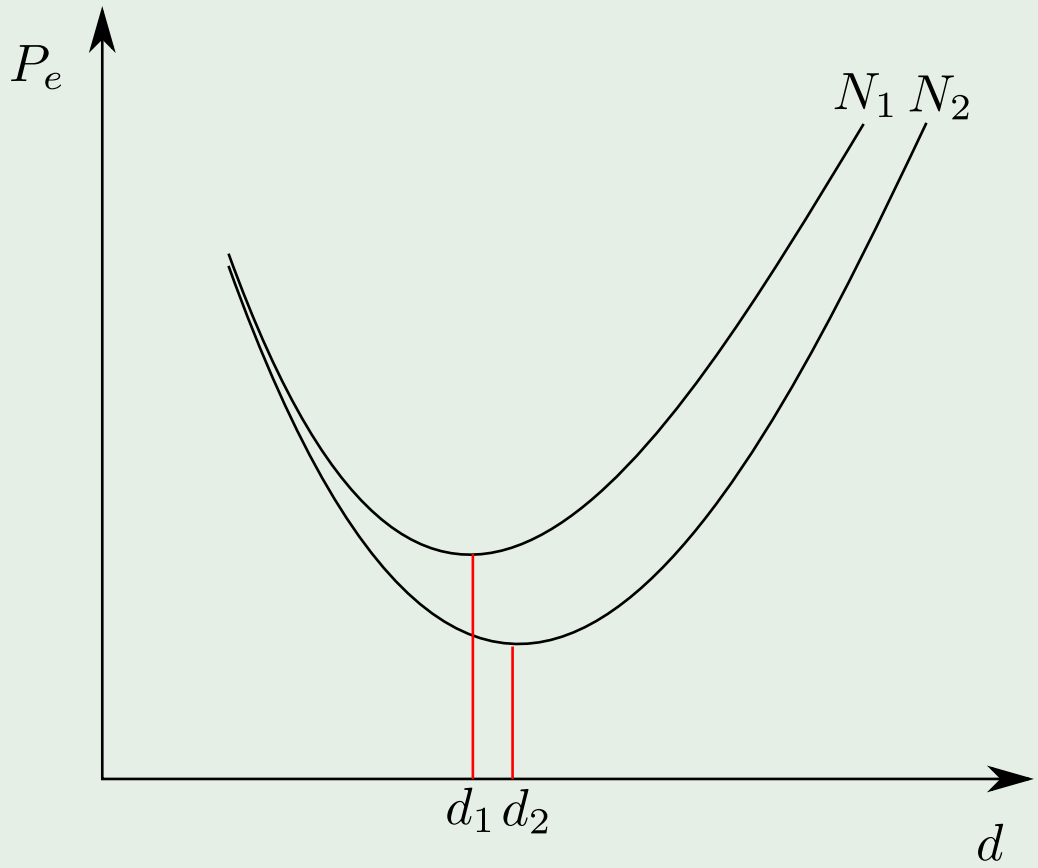
- If the PDF's are not known, then the arbitrary increase of the number of features leads to the maximum possible value of the error rate, that is, $\frac{1}{2}$.

Thus

- Under a limited number of training data we must try to keep the number of features to a relatively low number.

Graphically

For $N_2 \gg N_1$, minimum at $d = \frac{N}{\alpha}$ with $\alpha \in [2, 10]$



Back to Feature Selection

The Goal

1. Select the "optimum" number d of features.

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Outline

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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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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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1. Discard individual features with poor information content.

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

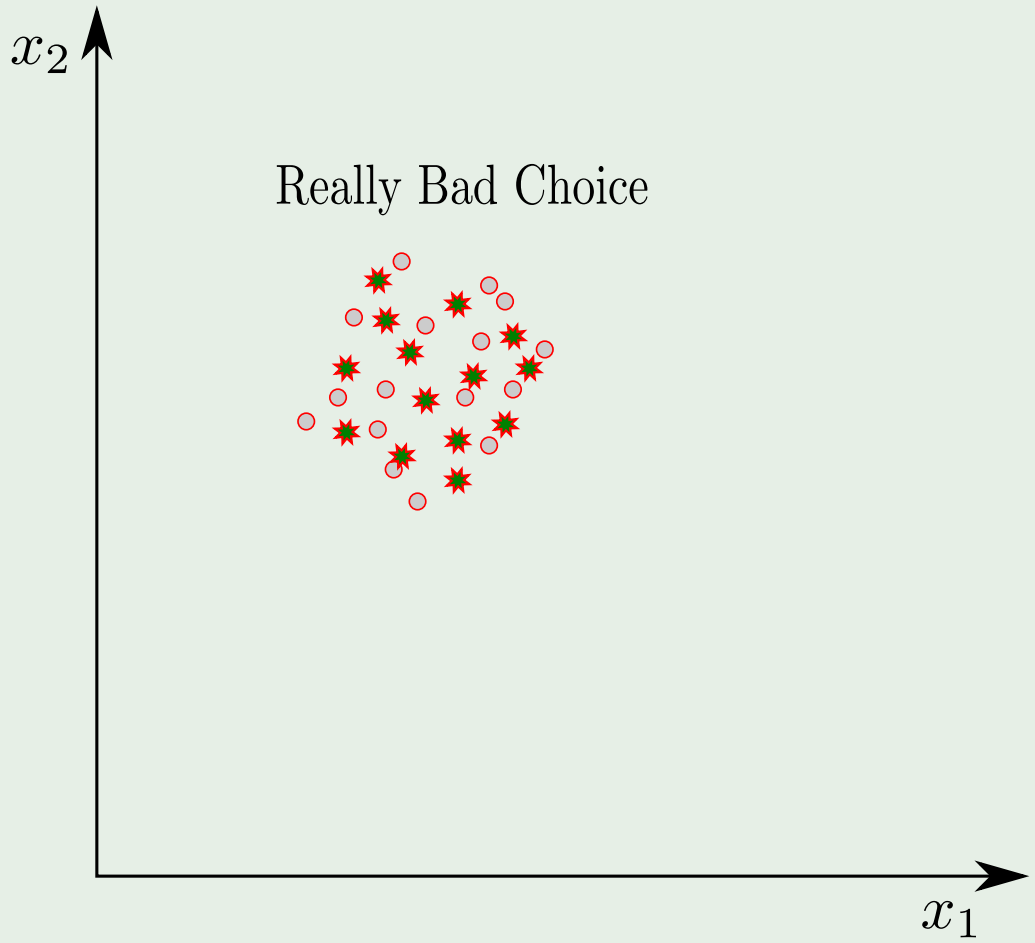
Best: Large between class distance, Small within class variance.

The basic philosophy

1. Discard individual features with poor information content.
2. The remaining information rich features are examined jointly as vectors

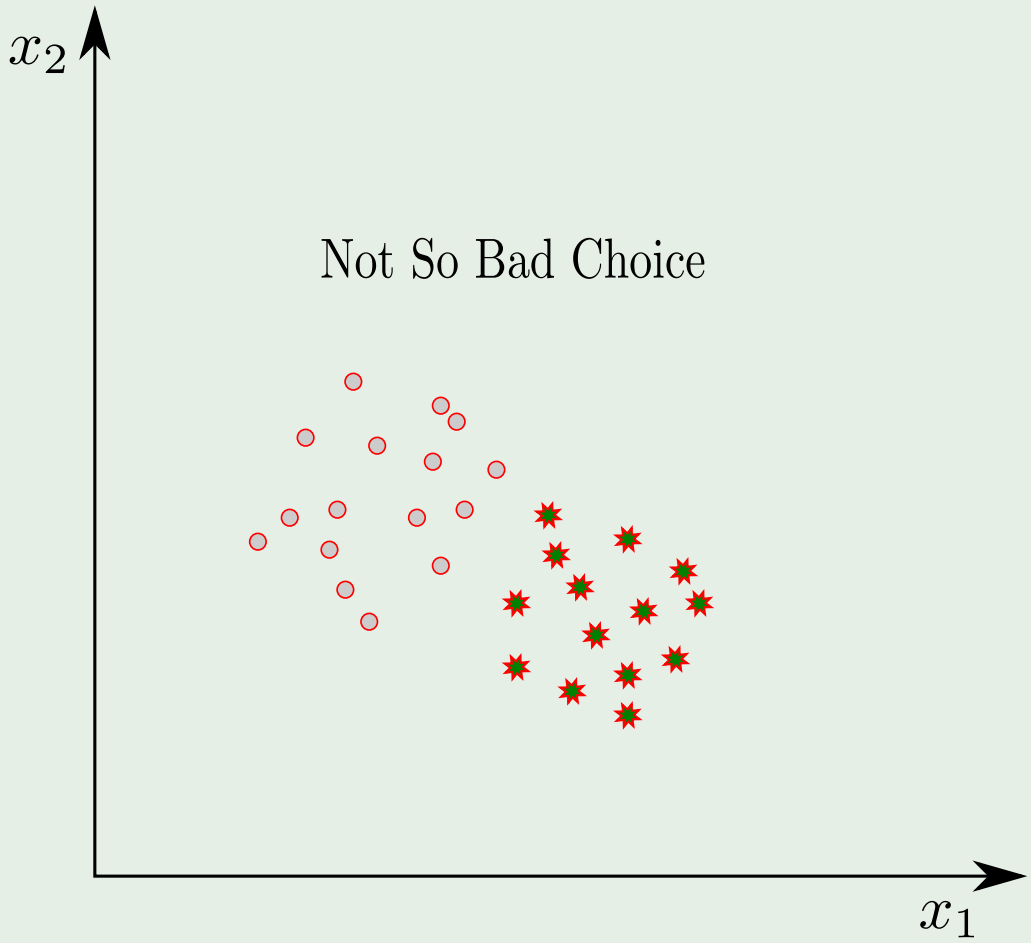
Example

Thus, we want to avoid choices



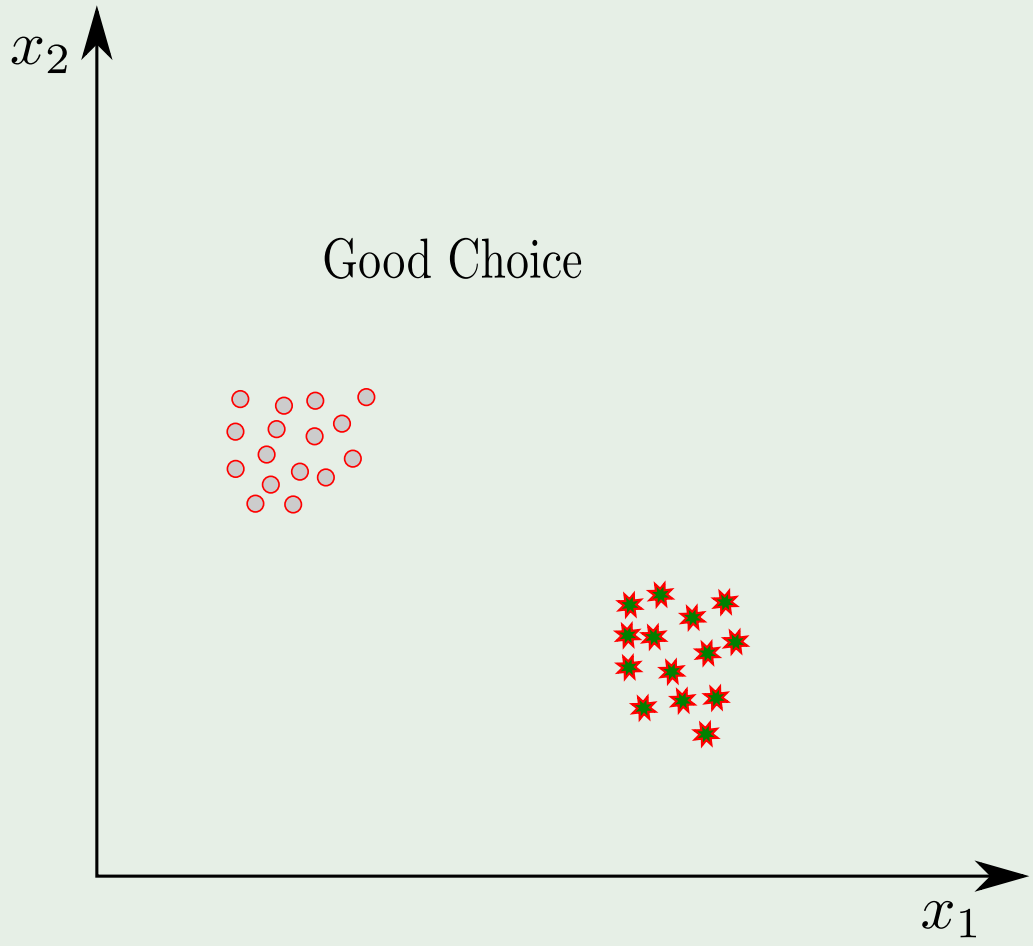
Example

Better Choice



Example

What We Want to Have



Outline

Using Statistics

Simplicity First Principles - Marcus Aurelius

- A first step in feature selection is to look at each of the generated features independently.

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Meaning

H_0 is known as the null hypothesis and H_1 as the alternative hypothesis.

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We need to represent these ideas in a more mathematical way

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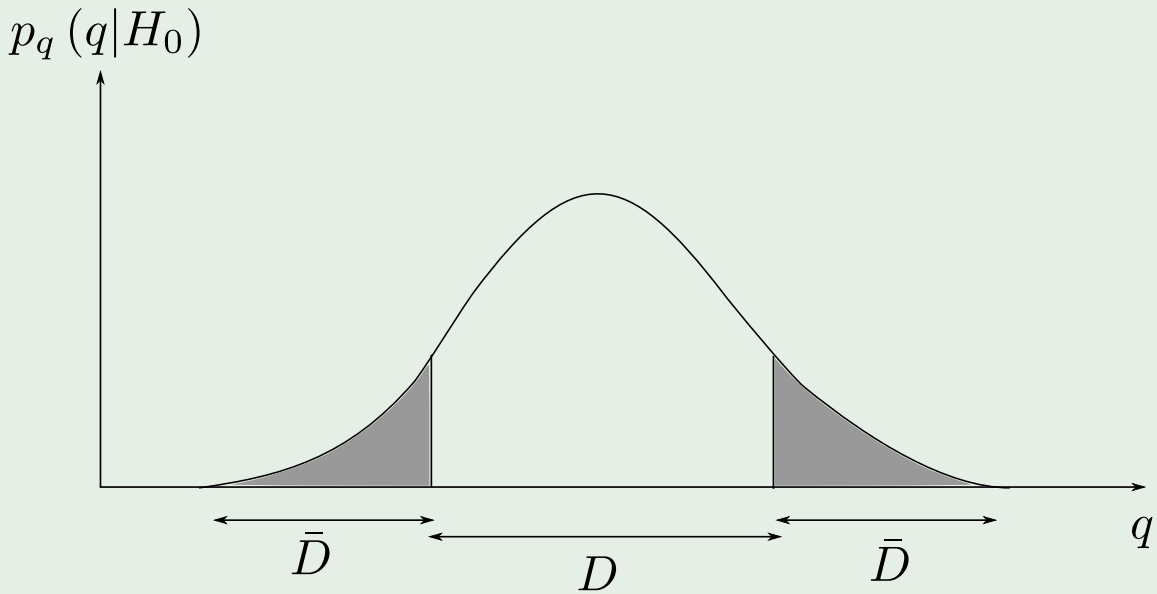
Example

Acceptance and critical regions for hypothesis testing. The area of the shaded region is the probability of an erroneous decision.



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We can estimate μ using

$$\overline{x} = \frac{1}{N}\sum_{i=1}^{N} x_i \tag{20}$$

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It can be proved that the

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The variance of $\sigma^2_{\overline{x}}$ of $\overline{x}$ is

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Which is the following

$$E\left[(\overline{x}-\mu)^2\right] = \frac{1}{N^2}\sum_{i=1}^{N} E\left[(x_i-\mu)^2\right] + \frac{1}{N^2}\sum_{i}\sum_{j\neq i} E\left[(x_i-\mu)(x_j-\mu)\right] \quad (22)$$

Known Variance Case

Because independence

$$E\left[(x_i - \mu)((x_j - \mu)\right] = E\left[x_i - \mu\right] E\left[x_j - \mu\right] = 0 \tag{23}$$

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Because independence

$$E\left[(x_i - \mu)((x_j - \mu)\right] = E\left[x_i - \mu\right] E\left[x_j - \mu\right] = 0 \tag{23}$$

Thus

$$\sigma_{\overline{x}}^2 = \frac{1}{N}\sigma^2 \tag{24}$$

Note: the larger the number of measurement samples, the smaller the variance of $\overline{x}$ around the true mean.

What to do with it

Now, you are given a $\widehat{\mu}$ the estimated parameter (In our case the mean sample)

Thus:

$$\begin{aligned} H_1 &: E[x] \neq \widehat{\mu} \\ H_0 &: E[x] = \widehat{\mu} \end{aligned}$$

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$$q = \frac{\overline{x} - \widehat{\mu}}{\frac{\sigma}{N}} \tag{25}$$

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Recalling the central limit theorem

The probability density function of $\overline{x}$ under H_0 is approx Gaussian $N\left(\widehat{\mu}, \frac{\sigma}{N}\right)$

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Then

We can choose an acceptance level ρ with interval $D = [-x_\rho, x_\rho]$ such that q lies on it with probability $1 - \rho$.

Final Process

First Step

- Given the N experimental samples of x, compute $\overline{x}$ and then q.

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- Choose the significance level ρ.

Third One

- Compute from the corresponding tables for $N(0,1)$ the acceptance interval $D = [-x_\rho, x_\rho]$ with probability $1 - \rho$.

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If $q \in D$ decide H_0 , if not decide H_1.

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- Basically, all we say is that we expect the resulting value q to lie in the high-percentage $1 - \rho$ interval.

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If $q \in D$ decide H_0 , if not decide H_1.

Second one

- Basically, all we say is that we expect the resulting value q to lie in the high-percentage $1 - \rho$ interval.
- If it does not, then we decide that this is because the assumed mean value is not "correct."

Outline

Example

Let us consider an experiment with a random variable x of $\sigma = 0.23$

- Assume N to be equal to 16 and $\overline{x} = 1.35$
- Adopt $\rho = 0.05$

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We will test if the hypothesis $\widehat{\mu} = 1.4$ is true

$$P\left\{-1.97 < \frac{\overline{x} - \widehat{\mu}}{0.23/4} < 1.97\right\} = 0.95$$

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$$P\left\{-1.97 < \frac{\overline{x} - \widehat{\mu}}{0.23/4} < 1.97\right\} = 0.95$$

Therefore, we accept the hypothesis

- We have $1.237 < \widehat{\mu} < 1.463$

Outline

Application of the t-Test in Feature Selection

Very Simple

Use the difference $\mu_1 - \mu_2$ for the testing.

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Basically, if we have two classes... we must see different $\mu's$.

Assume that the variance of the feature values is the same in both

$$\sigma_1^2 = \sigma_2^2 = \sigma^2 \tag{26}$$

What is the Hypothesis?

A very simple one

$$\begin{aligned} H_1 &: \Delta\mu = \mu_1 - \mu_2 \neq 0 \\ H_0 &: \Delta\mu = \mu_1 - \mu_2 = 0 \end{aligned}$$

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where x, y denote the random variables corresponding to the values of the feature in the two classes.

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Properties

- $E[z] = \mu_1 - \mu_2$
- $\sigma_z^2 = 2\sigma^2$

Then

It is possible to prove that z follows the distribution

$$N\left(\mu_1 - \mu_2, \frac{2\sigma^2}{N}\right) \tag{28}$$

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where

$$s_z^2 = \frac{1}{2N-2}\left(\sum_{i=1}^{N}(x_i - \overline{x})^2 + \sum_{i=1}^{N}(y_i - \overline{y})^2\right) \tag{30}$$

Now

It can be shown that $\frac{s_z^2(2N-2)}{\sigma^2}$ follows

- A Chi-Square distribution with $2N-2$ degrees of freedom.

Now

It can be shown that $\frac{s_z^2(2N-2)}{\sigma^2}$ follows

- A Chi-Square distribution with $2N-2$ degrees of freedom.

Testing

- q turns out to follow a Chi-Square distribution with $2N-2$ degrees of freedom

Outline

We have two classes

The sample measurements of a feature in two classes are

class ω_1	3.5	3.7	3.9	4.1	3.4	3.5	4.1	3.8	3.6	3.7
class ω_2	3.2	3.6	3.1	3.4	3.0	3.4	2.8	3.1	3.3	3.6

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Now, we want to know if the feature is informative enough

$$\begin{aligned} H_1 &: \Delta\mu = \mu_1 - \mu_2 \neq 0 \\ H_0 &: \Delta\mu = \mu_1 - \mu_2 = 0 \end{aligned}$$

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Again, we choose $\rho = 0.05$

$$\begin{aligned} \omega_1 &: \overline{x} = 3.73,\ \widehat{\sigma}_1^2 = 0.0601 \\ \omega_2 &: \overline{y} = 3.25,\ \widehat{\sigma}_2^2 = 0.0672 \end{aligned}$$

Then

For $N = 10$

- $s_z^2 = \frac{1}{2}\left(\widehat{\sigma}_1^2 + \widehat{\sigma}_2^2\right)$
- $q = \frac{(\overline{x} - \overline{y} - 0)}{s_z \sqrt{\frac{2}{N}}}$

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We have $q = 4.25$

- We have 20-2 $=$ 18 degrees of freedom and significance level 0.05

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Then, $D = [-2.10, 2.10]$

- $q = 4.25$ is outside of D, we decide $H_1 : \Delta\mu = \mu_1 - \mu_2 \neq 0$

Finally

The means μ_1 and μ_2 are significantly different with $\alpha = 0.05$

- The Feature is selected

Outline

Considering Feature Sets

Something Notable

- The emphasis so far was on individually considered features.

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But

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Then

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

What to do?

Possible

- Use different feature combinations to form the feature vector.

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However

- A major disadvantage of this approach is the high complexity.
- Also, local minimum may give misleading results.

Better

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

Outline

Scatter Matrices

Definition

- These are used as a measure of the way data are scattered in the respective feature space.

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Within-class Scatter Matrix

$$S_w = \sum_{i=1}^{C} P_i S_i \tag{31}$$

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    1. n_i is the number of samples in class ω_i.

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Between-class scatter matrix

$$S_b = \sum_{i=1}^{C} P_i \left(\boldsymbol{x} - \boldsymbol{\mu_0}\right) \left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T \tag{32}$$

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The global mean.

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Where

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The global mean.

Mixture scatter matrix

$$S_m = E\left[\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)\left(\boldsymbol{x} - \boldsymbol{\mu_0}\right)^T\right] \tag{34}$$

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

Criterion's

First One

$$J_1 = \frac{trace\{S_m\}}{trace\{S_w\}} \tag{35}$$

- 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.

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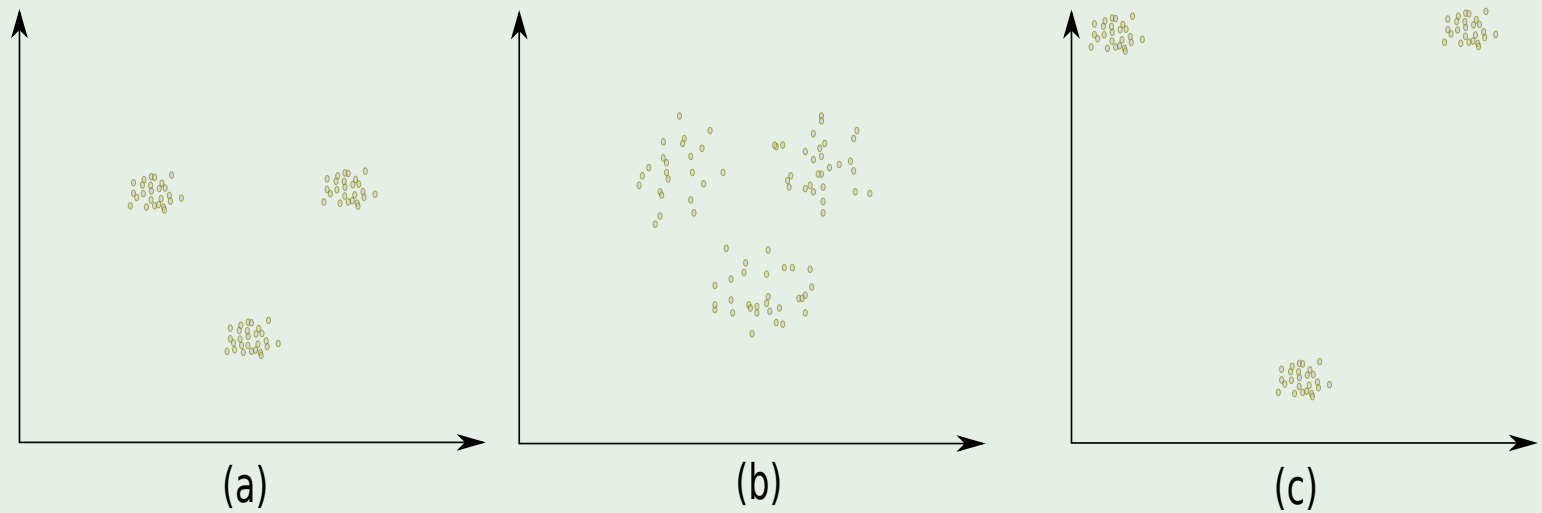
1. $J_2 = \frac{|S_m|}{|S_w|}$
2. $J_3 = trace\{S_w^{-1} S_m\}$

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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1. Select a class separability
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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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

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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

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

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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Use criterion C

To select the best one

Complexity of the Method

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Thus, starting from m, at each step we drop out one feature from the "best" combination until we obtain a vector of l features.

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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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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

Shrinkage Methods

By retaining a subset of the predictors and discarding the rest

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However given process

- it often exhibits high variance,
- It does not reduce the prediction error of the full model.

Therefore

- Shrinkage methods are more continuous avoiding high variability.

Outline

The house example

Imagine the following data set

Now assume that we use LSE

For the fitting

$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{w}}\left(x_i\right)-y_i\right)^2$$

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$$\frac{1}{2}\sum_{i=1}^{N}\left(h_{\boldsymbol{w}}\left(x_i\right)-y_i\right)^2$$

We can then run one of our machine to see what minimize better the previous equation

Question: Did you notice that I did not impose any structure to $h_{\boldsymbol{w}}\left(x\right)$?

Then, First fitting

What about using $h_1(x) = w_0 + w_1 x + w_2 x^2$?

Second fitting

What about using $h_2(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4 + w_5 x^5$?

Therefore, we have a problem

We get weird overfitting effects!!!

What do we do? What about minimizing the influence of w_3, w_4, w_5?

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What do we do? What about minimizing the influence of w_3, w_4, w_5?

How do we do that?

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}} \left(x_i \right) - y_i \right)^2$$

What about integrating those values to the cost function? Ideas

Outline

We have

Regularization intuition is as follow

Small values for parameters $w_0, w_1, w_2, ..., w_n$

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Small values for parameters $w_0, w_1, w_2, ..., w_n$

It implies

1. "Simpler" function
2. Less prone to overfitting

We can do the previous idea for the other parameters

We can do the same for the other parameters

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}} \left(x_i \right) - y_i \right)^2 + \sum_{i=1}^{d} \lambda_i w_i^2 \tag{36}$$

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However handling such many parameters can be so difficult

Combinatorial problem in reality!!!

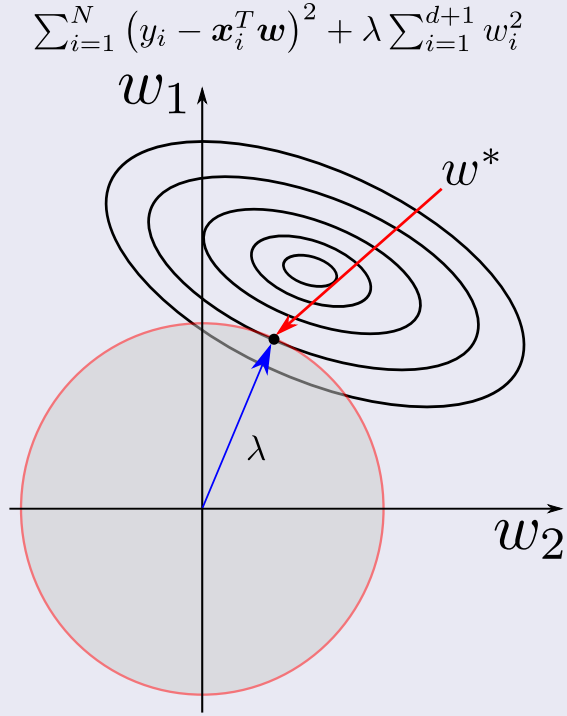
Better, we can

We better use the following

$$\min_{\boldsymbol{w}} \frac{1}{2} \sum_{i=1}^{N} \left(h_{\boldsymbol{w}} \left(x_i \right) - y_i \right)^2 + \lambda \sum_{i=1}^{d} w_i^2 \tag{37}$$

Graphically

Geometrically Equivalent to



Outline

Ridge Regression

Equation

$$\widehat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left(y_i - w_0 - \sum_{j-1}^{d} x_{ij} w_j \right)^2 + \lambda \sum_{j=1}^{d} w_j^2 \right\}$$

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Here

- $\lambda \geq 0$ is a complexity parameter that controls the amount of shrinkage

Therefore

The Larger $\lambda \geq 0$

- The coefficients are shrunk toward zero (and each other).

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This is also used in Neural Networks

- where it is known as weight decay

This is also can be written

Optimization Solution

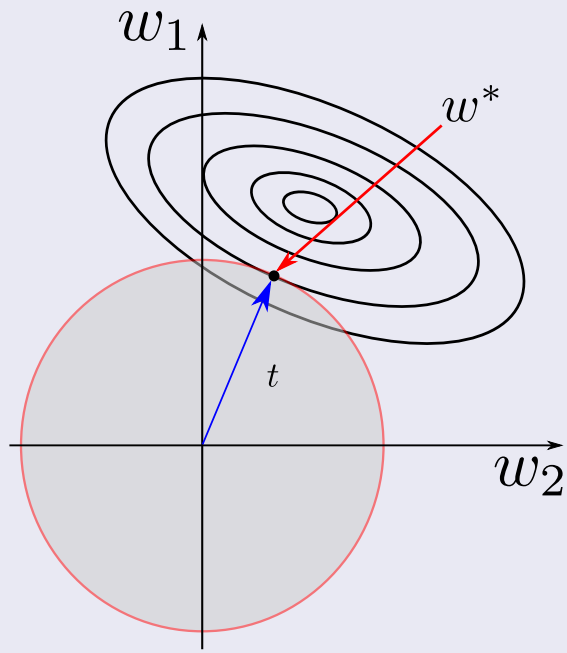
$$\arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left(y_i - w_0 - \sum_{j-1}^{d} x_{ij} w_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{d} w_j^2 < t$$

Graphically

Geometrically Equivalent to

$$\begin{aligned} &\arg\min \ \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{w}\right)^2 \\ &\text{subject to } \sum_{i=1}^{d+1} w_i^2 < t \end{aligned}$$



Outline

Remarks

We have the following

- The Ridge solutions are not equivariant under scaling of the inputs.

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Thus, the need to standardize the input data

- Before Solving the optimization:

$$\arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left(y_i - w_0 - \sum_{j-1}^{d} x_{ij} w_j \right)^2$$

$$\text{subject to } \sum_{j=1}^{d} w_j^2 < t$$

Here

Notice that w_0 is not being penalized

- Penalizing w_0 would make the procedure depend on the origin chosen for y_i.

Therefore

We can center the Data

- Thus, each x_{ij} gets replaced by $x_{ij} - \bar{x}_j$.

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Then, we estimate w_0

$$w_0 = \frac{1}{N}\sum_{i=1}^{N} y_i$$

Thus after centering the Data

Now, Given a data matrix $\boldsymbol{X}$ with d dimensions

$$Loss_{RSS}(\lambda) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

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$$Loss_{RSS}(\lambda) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

The Ridge Regression solution is equivalent to

$$\widehat{\boldsymbol{w}}^{Ridge} = \left(\boldsymbol{X}^T \boldsymbol{X} + \lambda I\right)^{-1} \boldsymbol{X}^T \boldsymbol{y}.$$

Outline

Least Absolute Shrinkage and Selection Operator (LASSO)

It was introduced by Robert Tibshirani in 1996 based on Leo Breiman's nonnegative garrote

$$\widehat{\boldsymbol{w}}^{garrote} = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{d} x_{ij} w_j \right)^2 + N\lambda \sum_{j=1}^{d} w_j$$

$$\text{s.t. } w_j > 0 \ \forall j$$

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Robert Tibshirani proposed the use of the L_1 norm

$$\|\boldsymbol{w}\|_1 = \sum_{i=1}^{d} |w_i|$$

The Final Optimization Problem

LASSO

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This is not derivable

More advanced methods are necessary to solve this problem!!!

Outline

The Lagrangian Version

The Lagrangian

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The Lagrangian Version

The Lagrangian

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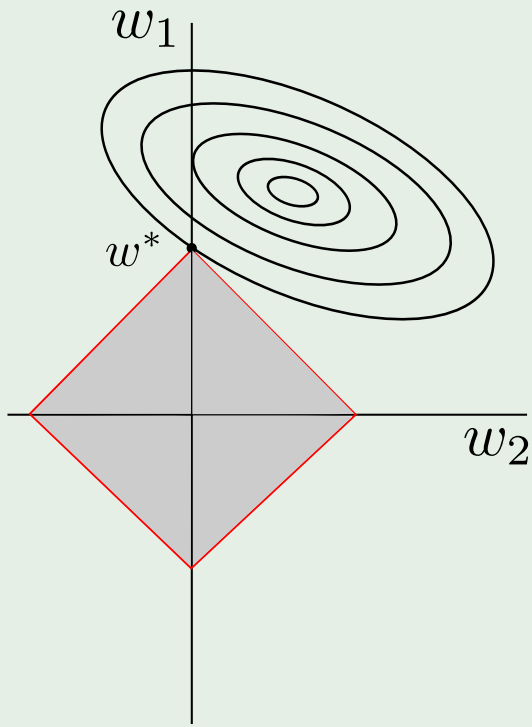
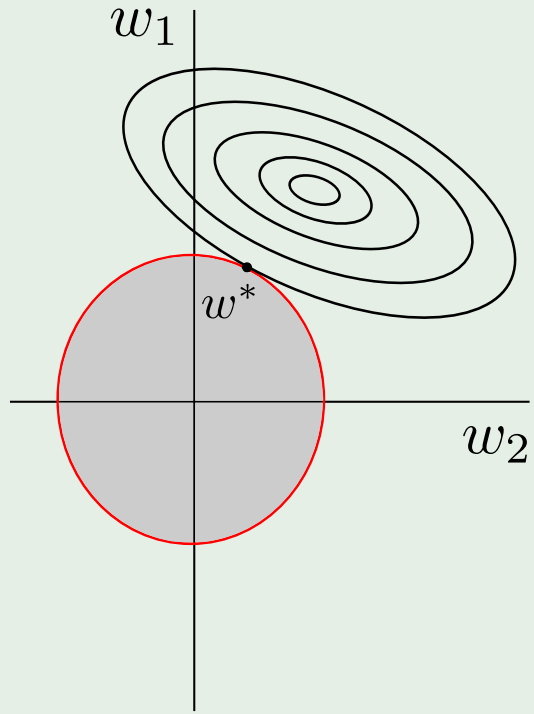
However

You have other regularizations as $\|\boldsymbol{w}\|_2 = \sqrt{\sum_{i=1}^{d} |w_i|^2}$

Graphically

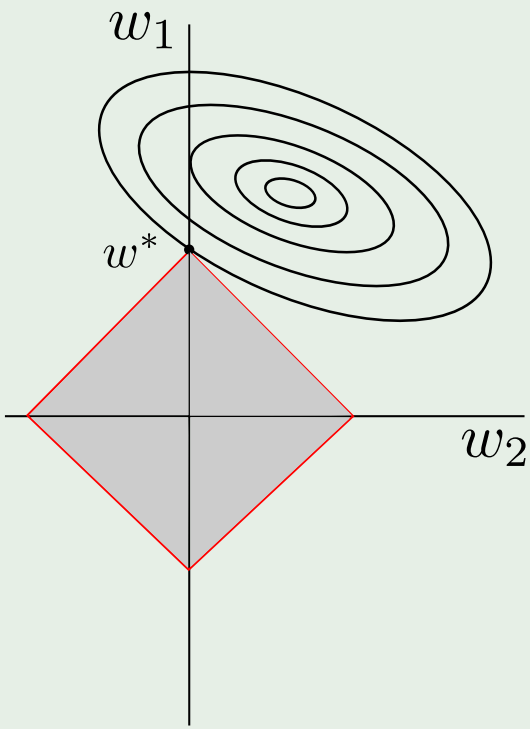
The first area correspond to the L_1 regularization and the second one?

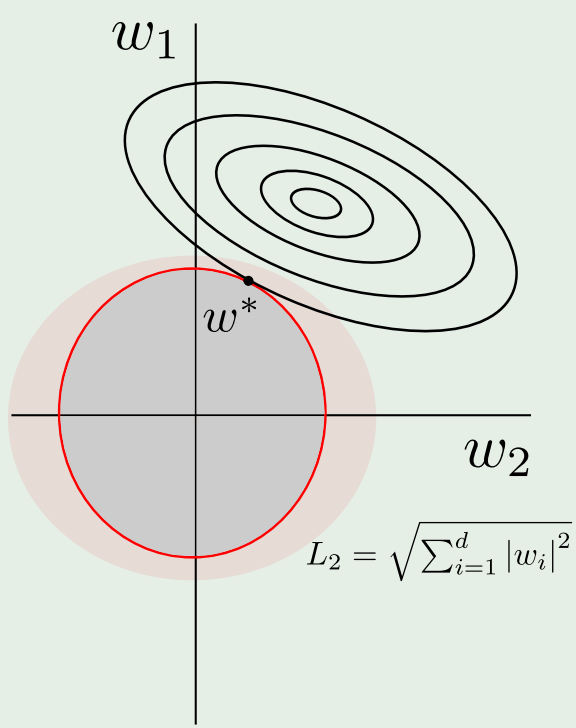




Graphically

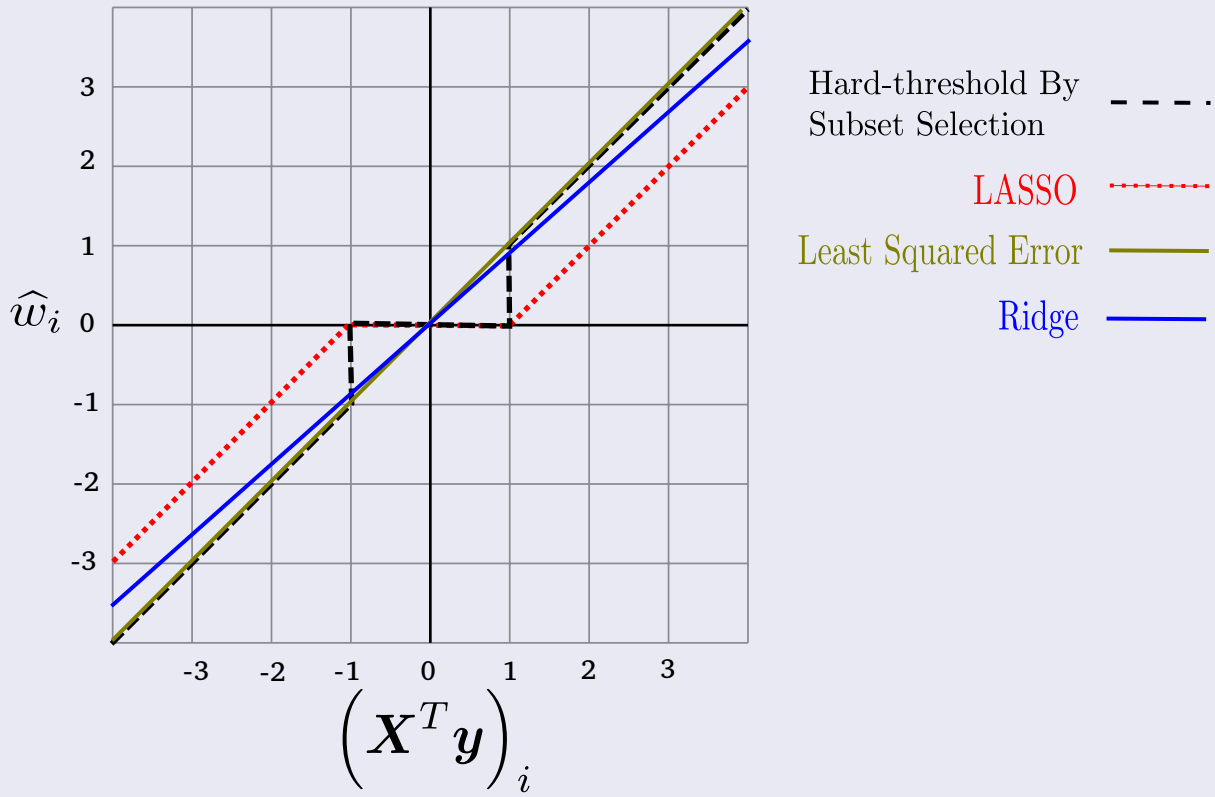
Yes the circle defined as $\|\boldsymbol{w}\|_2 = \sqrt{\sum_{i=1}^{d} |w_i|^2}$





For Example

In the Case of $\boldsymbol{X}$ is a Orthogonal Matrix



The seminal paper by Robert Tibshirani

An initial study of this regularization can be seen in

"Regression Shrinkage and Selection via the LASSO" by Robert Tibshirani - 1996

This out the scope of this class

However, it is worth noticing that the most efficient method for solving LASSO problems is

"Pathwise Coordinate Optimization" By Jerome Friedman, Trevor Hastie, Holger Ho and Robert Tibshirani

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Nevertheless

It will be a great seminar paper!!!

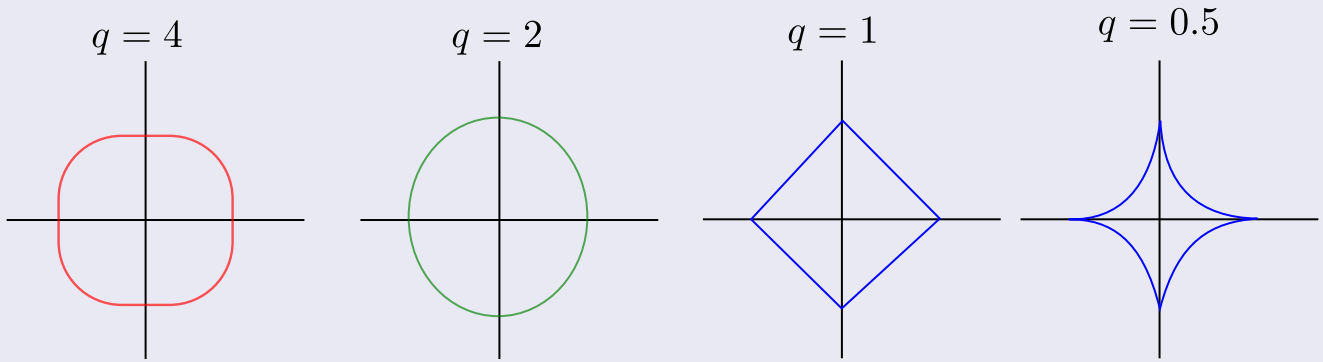
Furthermore

We can generalize ridge regression and the lasso, and view them as Bayes estimates

$$\widehat{\boldsymbol{w}}^{LASSO} = \arg\min_{\boldsymbol{w}} \left\{ \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}^T \boldsymbol{w} \right)^2 + \lambda \sum_{i=1}^{d} |w_i|^q \right\} \text{ with } q \geq 0$$

For Example

We have when $d = 2$



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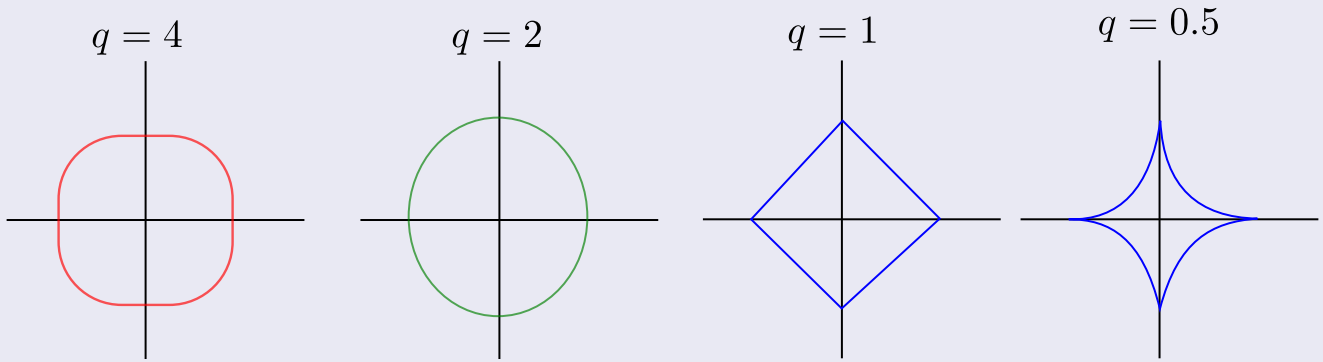

Here, when $q > 1$

- You are having a derivable Lagrangian, but you lose the LASSO properties

Therefore

Zou and Hastie (2005) introduced the elastic- net penalty

$$\lambda \sum_{i=1}^{d} \left\{ \alpha w_i^2 + (1-\alpha) |w_i| \right\}$$

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$$\lambda \sum_{i=1}^{d} \left\{ \alpha w_i^2 + (1-\alpha) |w_i| \right\}$$

This is Basically

- A Compromise Between the Ridge and LASSO.