Introduction to Machine Learning

Feature Selection

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June 14, 2020

Outline

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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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Why is important?

1. If we selected features with little discrimination power, the subsequent design of a classifier would lead to poor performance.
2. if information-rich features are selected, the design of the classifier can be greatly simplified.

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

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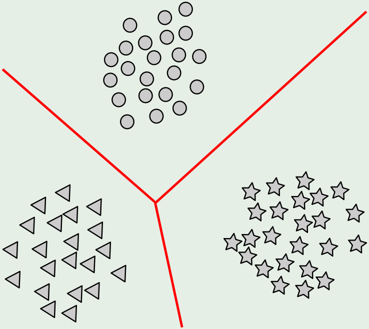
Then

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



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It is necessary to do the following

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

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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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For a normally distributed random

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

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Then removing outliers is the biggest importance.

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You can do the following

1. If you have a small number $\Rightarrow$ discard them!!!
2. Adopt cost functions that are not sensitive to outliers:
   1. For example, possibilistic clustering.
3. For more techniques look at
   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

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

$$\chi_d^2(0.05)$$

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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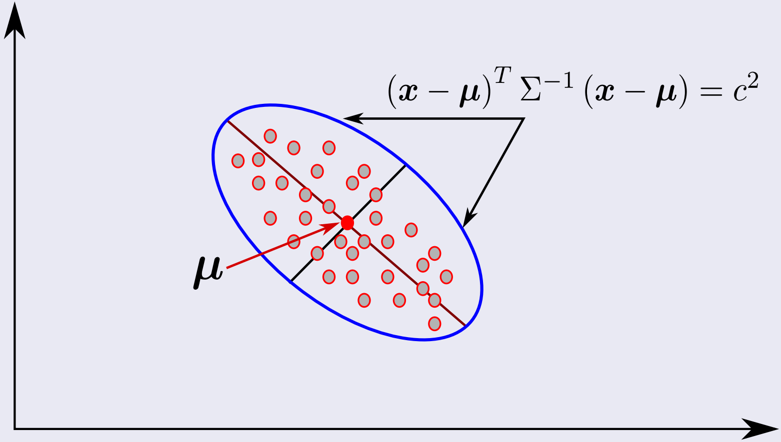
Mahalonobis Distance

We have

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

Thus

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



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

The solid ellipsoid of x vectors satisfying

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

has a probability $1-\alpha$.

How?

We know that

χ_d^2 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.

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

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

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Something Notable

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

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

We have

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

Then

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

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Therefore

If we define

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

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

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

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Therefore

We have that $Z_1, Z_2, \ldots, Z_d$ 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 $N_d(\boldsymbol{\mu}, \Sigma)$

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

Basically $\chi_d^2(\alpha)$ 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!!!

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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)
```

Outline

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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We have the following situation

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

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

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

Problem

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

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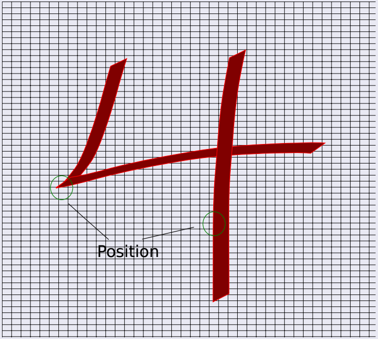
However

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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Thus

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

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

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Gaussian Mehtod

Thus

- All new features have zero mean and unit variance.

Further

- 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.

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Soft Max Scaling

Softmax Scaling

- It consists of two steps

First one

$$y_{ik} = \frac{x_{ik} - \overline{x}_k}{\sigma} \qquad (3)$$

Second one

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

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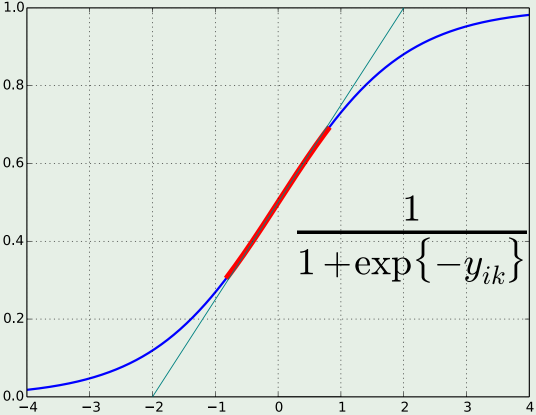
Explanation

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.

And values too away from the mean

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

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.

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

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

Outline

Missing Data

This can happen

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

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Examples where this happens

1. Social sciences - incomplete surveys.
2. Remote sensing - sensors go off-line.
3. etc.

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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

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

Find the distribution of your data

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

$$\overline{x}_i = \frac{\alpha}{\alpha+\beta} \quad (7)$$

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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

Something more advanced

Split data samples in two set of variables

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

Generate the following probability distribution

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

where

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

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We can use EM

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 $x_{missed} \sim p_j\left(x|\theta\right) + Var\left(x\right)$

This is the most simple

- What about something more complex?

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This is the most simple

- What about something more complex?

For this, we can do

We have the following joint probability

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

Thus, the complete log likelihood

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

Therefore, we have

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

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Here, it is quite interesting

We have a ratio like this

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

Basically we can get the Q function

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

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In this case

Why this ratio?

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

Actually... There is something quite interesting

- Kullback–Leibler Divergence!!!

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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

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

Thus, we have that

$$Q\left(\theta|\theta_t\right) = \int \log\frac{f\left(x_{missed}, x_{observed}|\theta\right)}{f\left(x_{missed}, x_{observed}|\theta_t\right)} f\left(x_{observed}|x_{missed}, \theta_t\right) dx_{observed}$$

$$= \int \log\frac{f\left(x_{observed}|x_{missed}, \theta\right) f\left(x_{missed}|\theta\right)}{f\left(x_{observed}|x_{missed}, \theta_t\right) f\left(x_{missed}|\theta_t\right)} f\left(x_{obser}|x_{missed}, \theta_t\right) dx_{obser}$$

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Basically, we have

The well known difference and KL Divergence

$$
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Q\left(\theta|\theta_t\right) = & \log f\left(\boldsymbol{x}_{missed}|\theta\right)\int f\left(\boldsymbol{x}_{observed}|\boldsymbol{x}_{missed},\theta_t\right)d\boldsymbol{x}_{observed} - \dots \\
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Using a little bit of notation

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

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

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It is possible to see that

Something Notable

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

Then

$$l_y\left(\theta_{t+1}\right) \geq l_y\left(\theta_t\right) + 0 + 0$$

Thus

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

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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!!!

Start from the simple

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

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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

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

Where, we have

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

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

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Incomplete observation

The likelihood function becomes

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

This is a quite unpleasant function

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

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What?

Let $X = \{X_1, ..., X_n\}$ be i.i.d. with $P(X_i = 1) = \alpha$

- Then, we play the hierarchical idea

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

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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

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

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Then taking logarithms

We have that

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

Therefore, if we differentiate

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

We have seen this formulations

- The EM algorithm for the Mixture of Gaussian's

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Outline

Example

We have two matrices

- Data Matrix X
- Missing Data M

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

Therefore, we have

- $X = (X_{obs}, X_{mis})$

This comes from

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

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We can use the following optimization

We can do the following

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

Clearly an initial matrix decomposition, where

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

So the total error to be minimized is

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

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- $K \ll N, M$

This can be regularized

Using the following ideas

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

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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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.

What?

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

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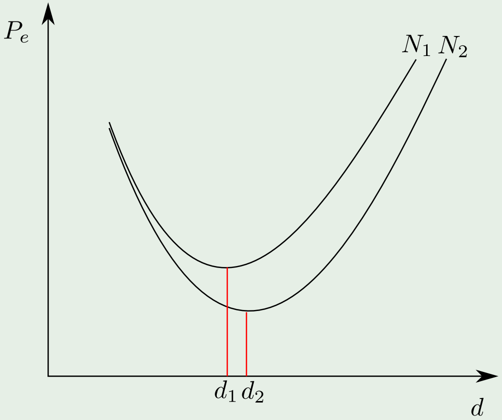
Graphically

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

THE PEAKING PHENOMENON

Assume the following problem

We have two classes ω_1, ω_2 such that

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

Both Classes have the following Gaussian distribution

1. $\omega_1 \Rightarrow \mu$ and $\Sigma = I$
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Where

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

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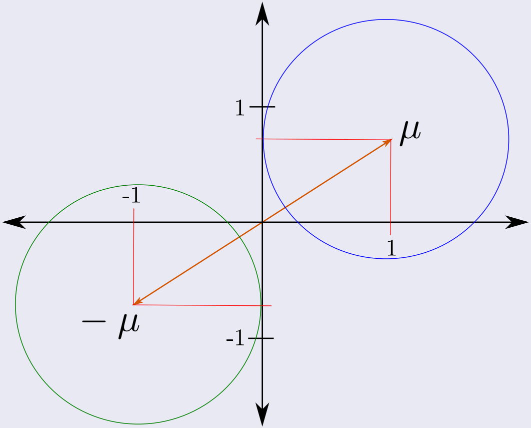
Example

The μ for $\mathbb{R}^2$

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



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A little bit of algebra

For the first case

$$\left\|\boldsymbol{x}-\boldsymbol{\mu}\right\|^2 < \left\|\boldsymbol{x}+\boldsymbol{\mu}\right\|^2$$

$$(\boldsymbol{x}-\boldsymbol{\mu})^T(\boldsymbol{x}-\boldsymbol{\mu}) < (\boldsymbol{x}+\boldsymbol{\mu})^T(\boldsymbol{x}+\boldsymbol{\mu})$$

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Given that z is a linear combination of independent Gaussian Variables

1. It is a Gaussian variable.
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Given that each feature of x

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Thus

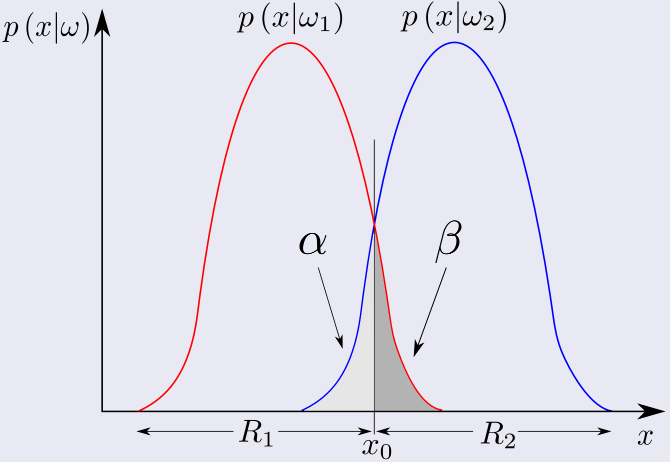
But, given that $x_i^2 \sim \chi_1^2\left(\frac{1}{i}\right)$, with mean

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

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

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

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

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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.

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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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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.

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, $\frac{1}{2}$.

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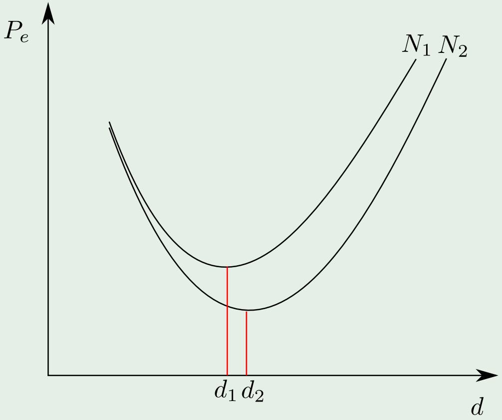
Graphically

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



Back to Feature Selection

The Goal

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Outline

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Given N

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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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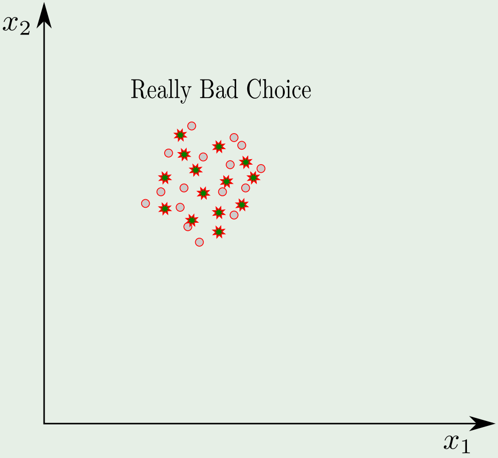
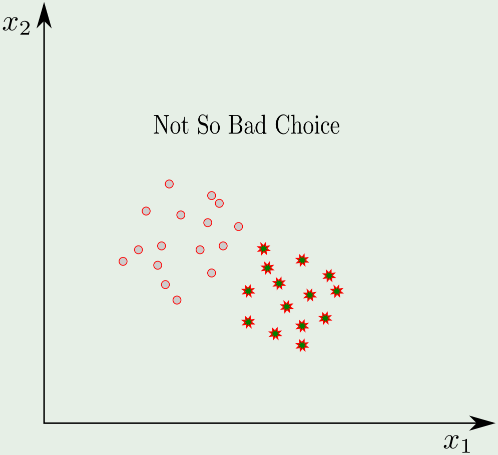
Example

Thus, we want to avoid choices



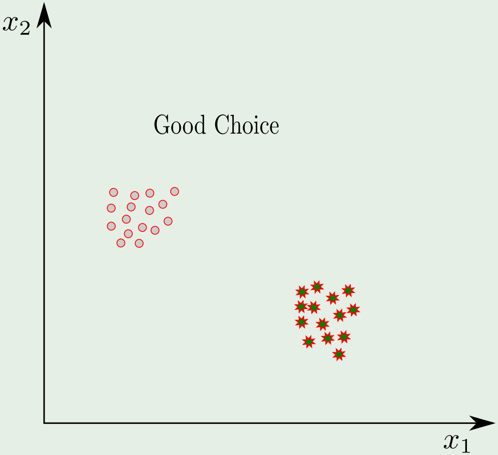
Example

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.
- Then, test their discriminatory capability for the problem at hand.

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We need to represent these ideas in a more mathematical way

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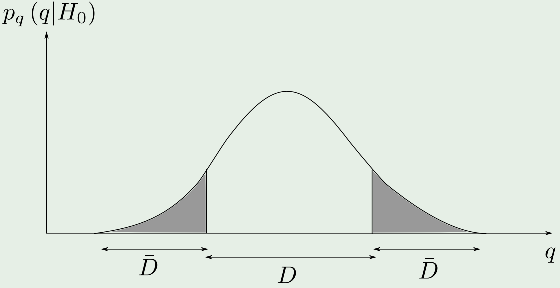
Example

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



Known Variance Case

Assume

Be x a random variable and x_i the resulting experimental samples.

Let

1. $E[x] = \mu$
2. $E\left[(x-\mu)^2\right] = \sigma^2$

We can estimate μ using

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

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In a similar way

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

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Which is the following

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

Recalling the central limit theorem

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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.

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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 $\rho = 0.05$

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

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

Therefore, we accept the hypothesis

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Application of the t -Test in Feature Selection

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A very simple one

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H_1 &: \Delta\mu = \mu_1 - \mu_2 \neq 0 \\
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The new random variable is

$$z = x - y \tag{27}$$

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

Properties

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It is possible to prove that z follows the distribution

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

So

We can use the following

$$q = \frac{(\overline{x} - \overline{y}) - (\mu_1 - \mu_2)}{s_z\sqrt{\frac{2}{N}}} \tag{29}$$

where

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

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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

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

$$H_1 : \Delta\mu = \mu_1 - \mu_2 \neq 0$$
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Again, we choose $\rho = 0.05$

$$\omega_1 : \overline{x} = 3.73,\ \hat{\sigma}_1^2 = 0.0601$$
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For $N = 10$

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

We have $q = 4.25$

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

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

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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.

But

- That is, two features may be rich in information, but if they are highly correlated we need not consider both of them.

Then

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

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Better

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

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- Also, local minimum may give misleading results.

Better

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

What to do?

Possible

- Use different feature combinations to form the feature vector.
- Train the classifier, and choose the combination resulting in the best classifier performance.

However

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

Better

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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

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

- where C is the number of classes.

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

Where

$$\boldsymbol{\mu_0} = \sum_{i=1}^{C} P_i \boldsymbol{\mu_i} \quad (33)$$

The global mean.

Mixture scatter matrix

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Criterion's

First One

$$J_1 = \frac{trace\left\{S_m\right\}}{trace\left\{S_w\right\}} \quad (35)$$

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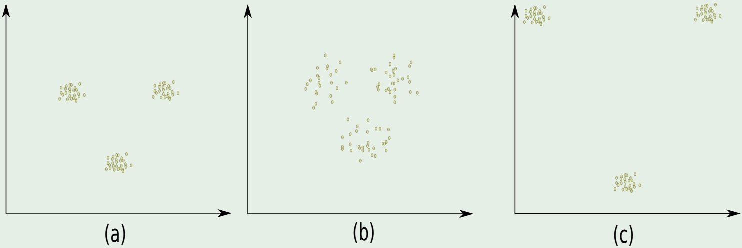
Example

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.



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We want to avoid

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As for example

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

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

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Eliminate one feature, you get

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

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- It suffers of the so-called nesting effect
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We can overcome this by using

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A more elegant methods are the ones based on

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Outline

Shrinkage Methods

By retaining a subset of the predictors and discarding the rest

- Subset Selection produces a model that is interpretable,
- It possibly produces lower prediction error than the full model.

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Outline

The house example

Imagine the following data set

Now assume that we use LSE

For the fitting

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

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 $h_w(x)$?

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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?

How do we do that?

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

What about integrating those values to the cost function? Ideas

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Regularization intuition is as follow

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

It implies

1. "Simpler" function
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However handling such many parameters can be so difficult

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We better use the following

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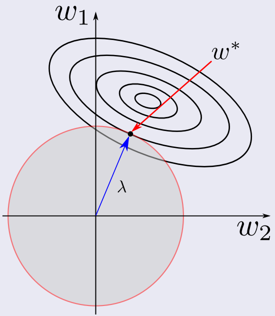
Graphically

Geometrically Equivalent to

$$\sum_{i=1}^{N}\left(y_i - \boldsymbol{x}_i^T\boldsymbol{w}\right)^2 + \lambda\sum_{i=1}^{d+1} w_i^2$$



Outline

Ridge Regression

Equation

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

Here

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

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Optimization Solution

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

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

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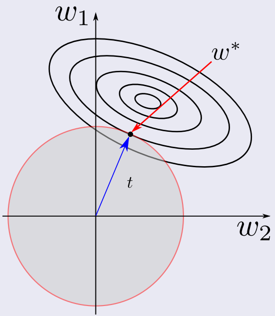

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as a number

We have

The ridge solutions are not equivariant under scaling of the inputs.

Thus, the need to standardize the input data

Before Solving:

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Thus after centering

Now the data matrix $\boldsymbol{X}$ has d dimensions

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

We have seen that the Ridge Regression solution is equivalent to

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

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Now

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We can define the degree of freedom by looking at the SVD, $\boldsymbol{X}$ $N \times d$

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T$$

With orthogonal matrices

1. The columns of $\boldsymbol{U}$ span the column space of $\boldsymbol{X}$
2. The columns of $\boldsymbol{V}$ span the row space of $\boldsymbol{X}$

And with $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0$ singular values

$$\boldsymbol{D} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \vdots \\ \vdots & 0 & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_d \end{pmatrix}$$

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Therefore, for the Ridge Regression

We have that

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

Thus, we have

$$\begin{aligned}\boldsymbol{X}\widehat{\boldsymbol{w}}^{Ridge} &= UDV^T\left(VDU^TUDV^T + \lambda VIV^T\right)VDU^T\boldsymbol{y} \\ &= UD\left(D^2 + \lambda I\right)^{-1}DU^T\boldsymbol{y}\end{aligned}$$

Finally

$$\boldsymbol{X}\widehat{\boldsymbol{w}}^{Ridge} = \sum_{i=1}^{d}\frac{\lambda_i^2}{\lambda_i^2 + \lambda}\boldsymbol{u}_i\boldsymbol{u}_i^T\boldsymbol{y}$$

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$$\begin{aligned}\boldsymbol{X}\widehat{\boldsymbol{w}}^{Ridge} &= \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T\left(\boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T + \lambda\boldsymbol{V}\boldsymbol{I}\boldsymbol{V}^T\right)\boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{y}\\ &= \boldsymbol{U}\boldsymbol{D}\left(\boldsymbol{D}^2 + \lambda I\right)^{-1}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{y}\end{aligned}$$

Finally

$$\boldsymbol{X}\widehat{\boldsymbol{w}}^{Ridge} = \sum_{i=1}^{d}\frac{\lambda_i^2}{\lambda_i^2 + \lambda}\boldsymbol{u}_i\boldsymbol{u}_i^T\boldsymbol{y}$$

Therefore

We have that given $\lambda \geq 0$

$$\frac{\lambda_i^2}{\lambda_i^2 + \lambda} \leq 1$$

Thus, like Linear Regression

- Ridge Regression computes the coordinates of y with respect to the orthonormal basis U.

Then, it shrinks the coordinates by a factor of $\frac{\lambda_i^2}{\lambda_i^2+\lambda}$

- Meaning the smaller is a λ_j the larger shrinkage you have!!!

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Therefore

This behaves has what we know as Principal Component Analysis

- We will look at this later...

Outline

Thus

Using Our Singular Value Decomposition

$$\boldsymbol{X}^T\boldsymbol{X} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{D}^2\boldsymbol{V}^T$$

Therefore the Sample Variance, for centered data, is defined as

$$C_X = \frac{1}{N}X^T X$$

Becomes which is called an eigen decomposition

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Goal of SVD

Find the best transformation with the minimal noise and redundancy

$$Y = \boldsymbol{X} A$$

Thus, we are looking by a orthonormal basis vectors

- Grouped as A

Covariance matrix captures all the information about X

- Only true for exponential family distributions

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First

Find the Covariance of Y

$$
\begin{aligned}
C_Y &= \frac{1}{N} Y^T Y \\
&= \frac{1}{N} (\boldsymbol{X} A)^T (\boldsymbol{X} A) \\
&= \frac{1}{N} A^T \boldsymbol{X}^T \boldsymbol{X} A
\end{aligned}
$$

Therefore

Find the direction for which the variance is maximized

$$v_1 = \arg\max_{v_1} \; var\left(Xv_1\right)$$
$$\text{s.t.} \;\; v_1^T v_1 = 1$$

We use the sample variance

$$var\left(Xv_1\right) = \frac{1}{N}\left(Xv_1\right)^T\left(Xv_1\right) = \frac{1}{N} v_1^T X^T X v_1 = v_1^T C_X v_1$$

Therefore

Find the direction for which the variance is maximized

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Thus

We have the Lagrangian

$$L\left(v_1, \lambda_1\right) = \boldsymbol{v}_1^T C_X \boldsymbol{v}_1 + \lambda_1 \left(1 - \boldsymbol{v}_1^T \boldsymbol{v}_1\right)$$

Thus, as in the PCA, $\boldsymbol{v}_1$ is an eigenvector of C_X

$$C_X \boldsymbol{v}_1 = \lambda_1 \boldsymbol{v}_1$$

With Variance

$$var\left(\boldsymbol{X}\boldsymbol{v}_1\right) = \boldsymbol{v}_1^T \frac{1}{N} V \boldsymbol{D}^2 V^T \boldsymbol{v}_1$$

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We have

$$var\left(X\boldsymbol{v}_1\right) = \frac{1}{N}\begin{bmatrix} 1 & 0 & \cdots & 0 \end{bmatrix}\begin{bmatrix} \lambda_1^2 & 0 & \cdots & 0 \\ 0 & \lambda_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_d^2 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

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Meaning

The First Principal Component Achieves maximum variance

- When the associated constant to the Sample Variance is equal to $\frac{\lambda_1^2}{N}$

In fact

We have that

$$\boldsymbol{z}_1 = \boldsymbol{X}\boldsymbol{v}_1 = \lambda_1 \boldsymbol{u}_1$$

This variable $\boldsymbol{z}_1$ is called the first principal component of $\boldsymbol{X}$

- Therefore $\boldsymbol{u}_1$ is called the normalized first principal component!!!

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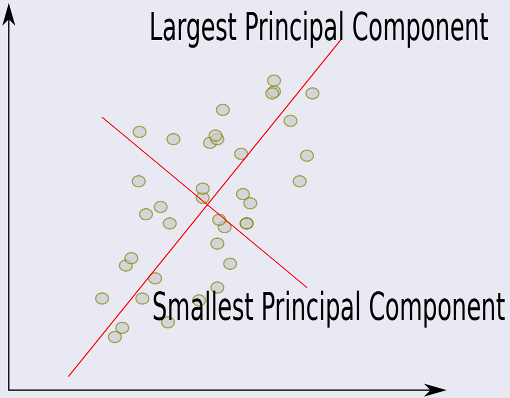
Geometrically

We have



We can define the following function

Effective Degrees of Freedom

About the Regularization Parameter λ

$$
\begin{aligned}
\text{df}(\lambda) =& tr\left[\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}+\lambda I\right)^{-1}\boldsymbol{X}^T\right]\\
=& tr\left[\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T\left(\boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T+\lambda I\right)^{-1}\boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\right]
\end{aligned}
$$

Therefore, the inner matrix

$$
\left(\boldsymbol{V}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T+\lambda I\right)^{-1}=\begin{pmatrix}
\frac{1}{\lambda_1^2+\lambda} & 0 & \cdots & 0\\
0 & \frac{1}{\lambda_2^2+\lambda} & \cdots & 0\\
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$$\mathrm{df}(\lambda) = tr\left[\boldsymbol{D}^2\left(\boldsymbol{D}^2+\lambda I\right)^{-1}\right] = tr\begin{pmatrix} \frac{\lambda_1^2}{\lambda_1^2+\lambda} & 0 & \cdots & 0 \\ 0 & \frac{\lambda_2^2}{\lambda_2^2+\lambda} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{\lambda_d^2}{\lambda_d^2+\lambda} \end{pmatrix}$$

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Degrees of Freedom in Linear Regression

Usually in a linear-regression fit with p variables

- The degrees-of-freedom of the fit is $d =$ number of features

This is important

- We assume all d coefficients in a ridge fit will be non-zero.
    - They are fit in a restricted fashion controlled by λ.

We have the following cases

- If $\mathrm{df}(\lambda) = d$ when $\lambda = 0$.
- If $\mathrm{df}(\lambda) \to 0$ as $\lambda \to \infty$

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From Hastie et. al page 63

Cancer Data using a Linear Model and df $(\lambda) = 5$

	LSE	Subset Selection	Ridge
Test Error	0.521	0.492	0.492
Std Error	0.179	0.143	0.1645

Outline

Least Absolute Shrinkage and Selection Operator (LASSO)

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

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

s.t. $w_j > 0 \ \forall j$

This is quite derivable

However, Tibshirani realized that you could get a more flexible model by using the absolute value at the constraint!!!

Robert Tibshirani proposed the use of the L_1 norm

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

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The Final Optimization Problem

LASSO

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Outline

The Lagrangian Version

The Lagrangian

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

However

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

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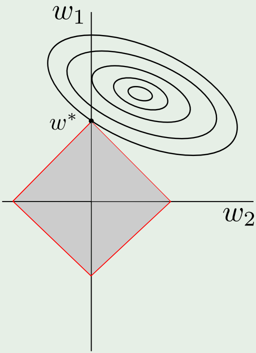
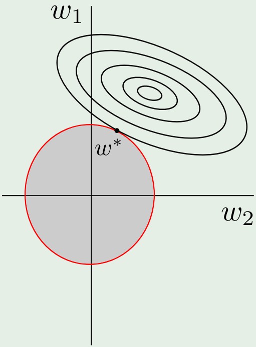
Graphically

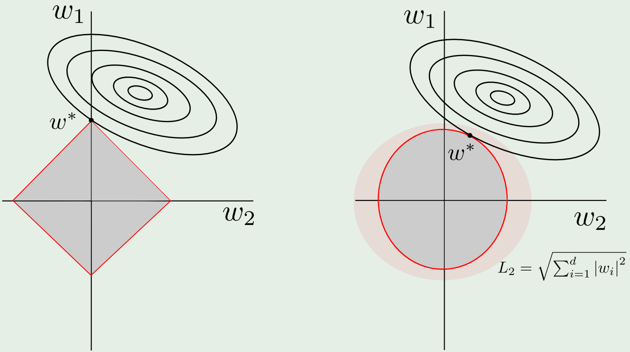
The first area correspond to the L_1 regularization and the second one?





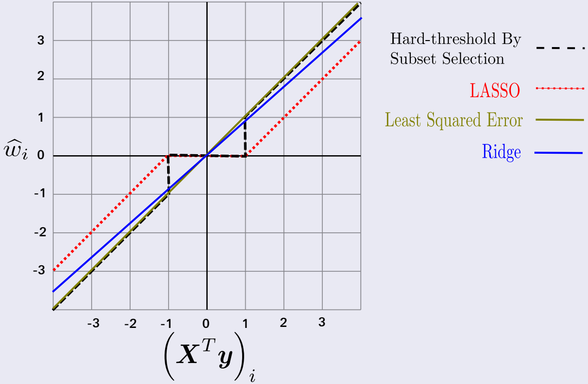
Graphically

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

Nevertheless

It will be a great seminar paper!!!

Generalization

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

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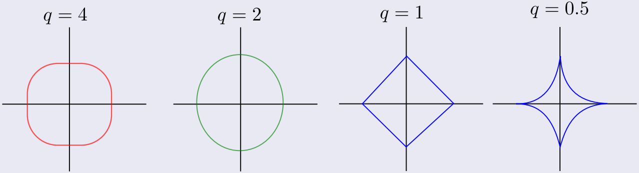
For Example

We have when $d = 2$



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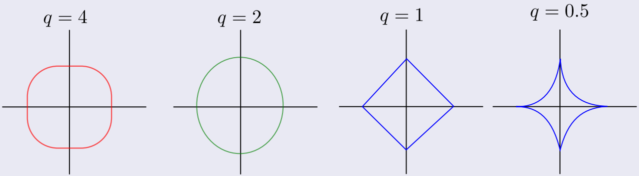

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Therefore

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

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

This is Basically

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