Introduction to Artificial Intelligence

Introduction to Linear Classifiers

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Outline

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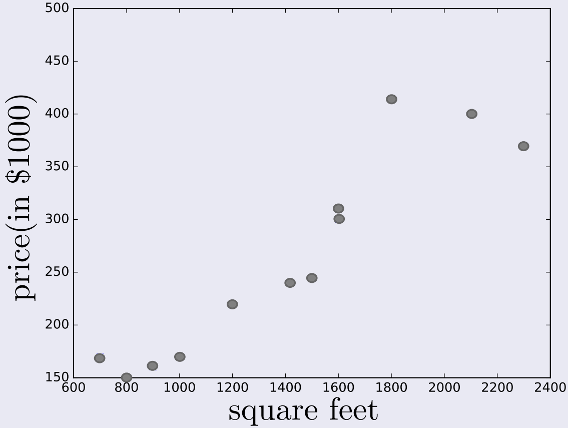
Many Times

We have this kind of data sets (House Prices)

$$\begin{pmatrix} \text{Squared Feet} \\ \text{Price} \end{pmatrix} \rightarrow \begin{pmatrix} 2104 \\ 400 \end{pmatrix} \begin{pmatrix} 1800 \\ 460 \end{pmatrix} \begin{pmatrix} 1600 \\ 300 \end{pmatrix} \begin{pmatrix} 2300 \\ 370 \end{pmatrix} \cdots$$



Thus

We can adjust a line/hyperplane to be able to forecast prices

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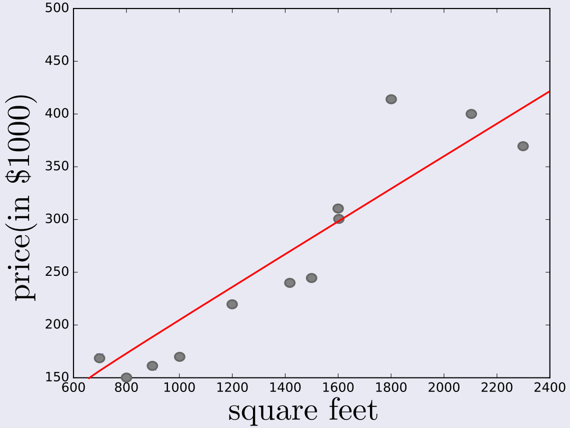

Thus, Our Objective

To find such hyperplane

To do forecasting on the prices of a house given its surface!!!

Here, where "Learning" Machine Learning style comes around

Basically, the process defined in Machine Learning!!!

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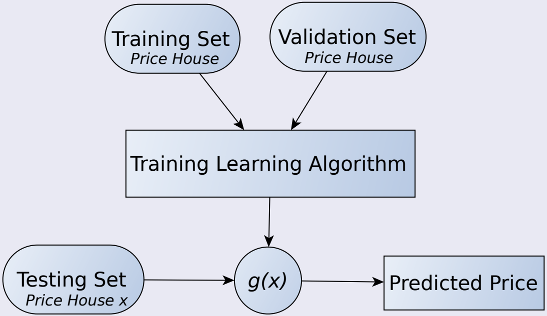
Then, in Supervised Training

We have the following process



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What is it?

First than anything, we have a parametric model!!!

Here, we have an hyperplane as a model:

$$g(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0 \tag{1}$$

Note: $\boldsymbol{w}^T\boldsymbol{x}$ is also know as dot product

In the case of $\mathbb{R}^2$

We have:

$$g(\boldsymbol{x}) = (w_1, w_2)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + w_0 = w_1x_1 + w_2x_2 + w_0 \tag{2}$$

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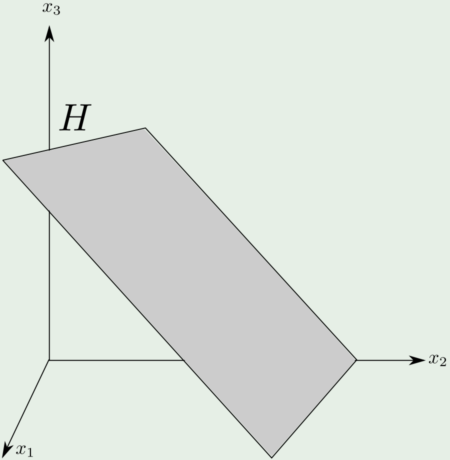
Example

Hyperplane in $\mathbb{R}^3$



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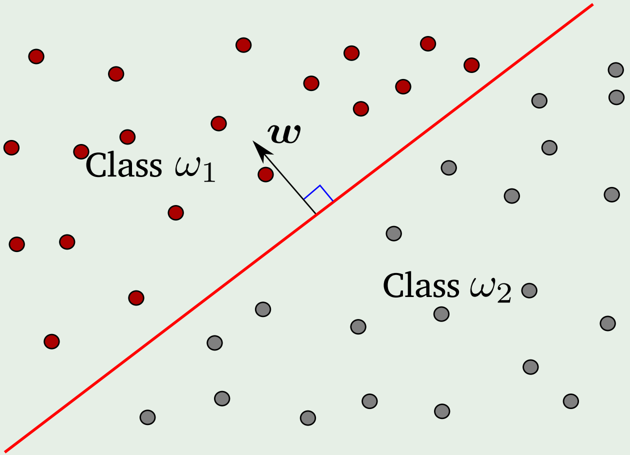
Splitting The Space $\mathbb{R}^2$

Using a simple straight line (Hyperplane)



Splitting the Space?

For example, assume the following vector $\boldsymbol{w}$ and constant w_0

$$\boldsymbol{w} = (-1, 2)^T \text{ and } w_0 = 0$$

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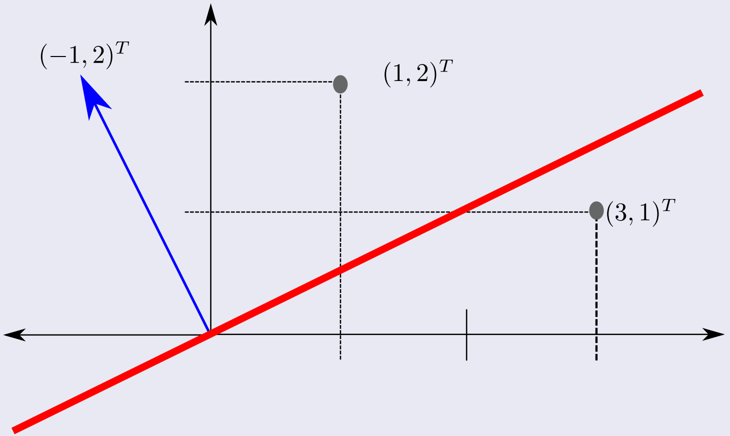

Then, we have

The following results

$$g\left(\begin{pmatrix} 1 \\ 2 \end{pmatrix}\right) = (-1, 2)\begin{pmatrix} 1 \\ 2 \end{pmatrix} = -1 \times 1 + 2 \times 2 = 3$$

$$g\left(\begin{pmatrix} 3 \\ 1 \end{pmatrix}\right) = (-1, 2)\begin{pmatrix} 3 \\ 1 \end{pmatrix} = -1 \times 3 + 2 \times 1 = -1$$

YES!!! We have a positive side and a negative side!!!

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The Decision Surface

The equation $g(x) = 0$ defines a decision surface

Separating the elements in classes, ω_1 and ω_2.

When $g(x)$ is linear the decision surface is an hyperplane

Now assume x_1 and x_2 are both on the decision surface

$$w^T x_1 + w_0 = 0$$
$$w^T x_2 + w_0 = 0$$

Thus

$$w^T x_1 + w_0 = w^T x_2 + w_0 \quad (3)$$

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Defining a Decision Surface

Then

$$\boldsymbol{w}^T\left(\boldsymbol{x}_1-\boldsymbol{x}_2\right)=0 \tag{4}$$

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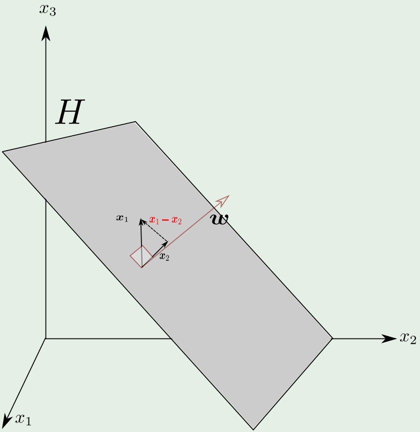
Therefore

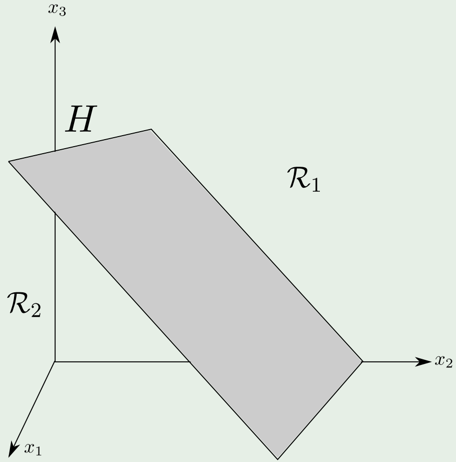
$x_1 - x_2$ lives in the hyperplane i.e. it is perpendicular to w^T

- Remark: any vector in the hyperplane is a linear combination of elements in a basis
- **Therefore any vector in the plane is perpendicular to w^T**



Therefore

The space is split in two regions (Example in $\mathbb{R}^3$) by the hyperplane H



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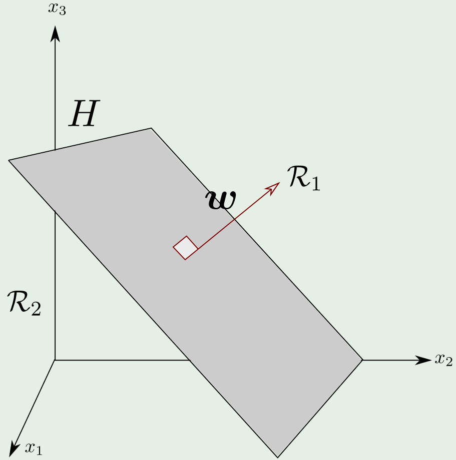
Some Properties of the Hyperplane

Given that $g(\boldsymbol{x}) > 0$ if $\boldsymbol{x} \in \mathcal{R}_1$



It is more

We can say the following

- Any $\boldsymbol{x} \in \mathcal{R}_1$ is on the positive side of H.
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In addition, $g(x)$ can give us a way to obtain the distance from x to the hyperplane H

First, we express any x as follows

$$x = x_p + r\frac{w}{\|w\|}$$

- r is the desired distance
  - Positive, if x is in the positive side
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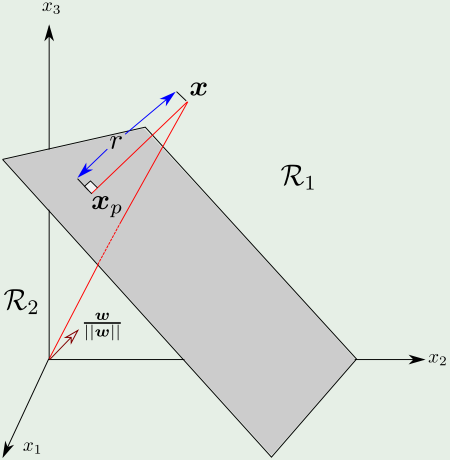
We have something like this

We have then



Now

Since $g(\boldsymbol{x}_p) = 0$

We have that

$$g(\boldsymbol{x}) = g\left(\boldsymbol{x}_p + r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}\right)$$

$$= \boldsymbol{w}^T\left(\boldsymbol{x}_p + r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}\right) + w_0$$

$$= \boldsymbol{w}^T\boldsymbol{x}_p + w_0 + r\frac{\boldsymbol{w}^T\boldsymbol{w}}{\|\boldsymbol{w}\|}$$

$$= g(\boldsymbol{x}_p) + r\frac{\|\boldsymbol{w}\|^2}{\|\boldsymbol{w}\|}$$

$$= r\|\boldsymbol{w}\|$$

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In particular

The distance from the origin to H

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Remarks

- If $w_0 > 0$, the origin is on the positive side of H.
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- If $w_0 = 0$, the hyperplane has the homogeneous form $w^T x$ and hyperplane passes through the origin.

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We want to solve the independence of w_0

We would like w_0 as part of the dot product by making $x_0 = 1$

$$g(\boldsymbol{x}) = w_0 \times 1 + \sum_{i=1}^{d} w_i x_i = w_0 \times x_0 + \sum_{i=1}^{d} w_i x_i = \sum_{i=0}^{d} w_i x_i \qquad (7)$$

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By making

$$x_{aug} = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{pmatrix} = \begin{pmatrix} 1 \\ \boldsymbol{x} \end{pmatrix}$$

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More Remarks

In addition

The hyperplane decision surface $\widehat{H}$ defined by

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passes through the origin in $\boldsymbol{x}_{aug}$-space.

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The distance from $\boldsymbol{y}$ to $\widehat{H}$ is:

$$\frac{\left|\boldsymbol{w}_{aug}^{T}\boldsymbol{x}_{aug}\right|}{\|\boldsymbol{w}_{aug}\|} = \frac{|g\left(\boldsymbol{x}_{aug}\right)|}{\|\boldsymbol{w}_{aug}\|}$$

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Now

Is $\|\boldsymbol{w}\| \leq \|\boldsymbol{w}_{aug}\|$

- Ideas?

$$\sqrt{\sum_{i=1}^{d} w_i^2} \leq \sqrt{\sum_{i=1}^{d} w_i^2 + w_0^2}$$

This mapping is quite useful

Because we only need to find a weight vector w_{aug} instead of finding the weight vector w and the threshold w_0.

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The name of this weight vector

It is called a separating vector or solution vector.

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We have a problem!!!

Which is the problem?

Now, assume the following

Imagine that your problem has two classes ω_1 and ω_2 in $\mathbb{R}^2$

1. They are linearly separable!!!
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A Simple Solution For Our Quandary

Label the Classes

- $\omega_1 \Longrightarrow +1$
- $\omega_2 \Longrightarrow -1$

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We produce the following labels

1. if $\boldsymbol{x} \in \omega_1$ then $y_{ideal} = g_{ideal}(\boldsymbol{x}) = +1$.
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Remark: We have a problem with this labels!!!

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Outline

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Now, What?

Assume true function f is given by

$$y_{noise} = g_{noise}(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + w_0 + e \quad (8)$$

Where the e

It has a $e \sim N(\mu, \sigma^2)$

Thus, we can do the following

$$y_{noise} = g_{noise}(\boldsymbol{x}) = g_{ideal}(\boldsymbol{x}) + e \quad (9)$$

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What to do?

$$e = y_{noise} - g_{ideal}\left(\boldsymbol{x}\right) \qquad (10)$$

Graphically

Thus, we have

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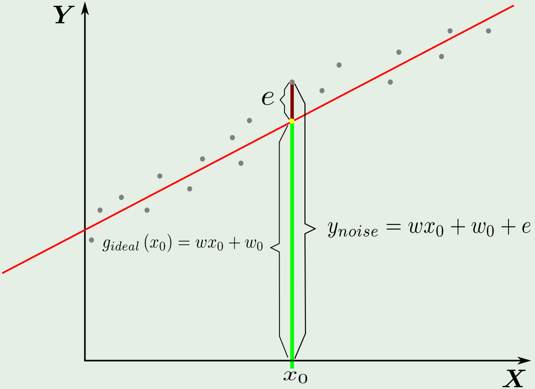
Graphically



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A TRICK... Quite a good one!!! Instead of using y_{noise}

$$e = y_{noise} - g_{ideal}(\boldsymbol{x}) \tag{11}$$

We use y_{ideal}

$$e = y_{ideal} - g_{ideal}(\boldsymbol{x}) \tag{12}$$

We will see

How the geometry will solve the problem with using these labels.

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Outline

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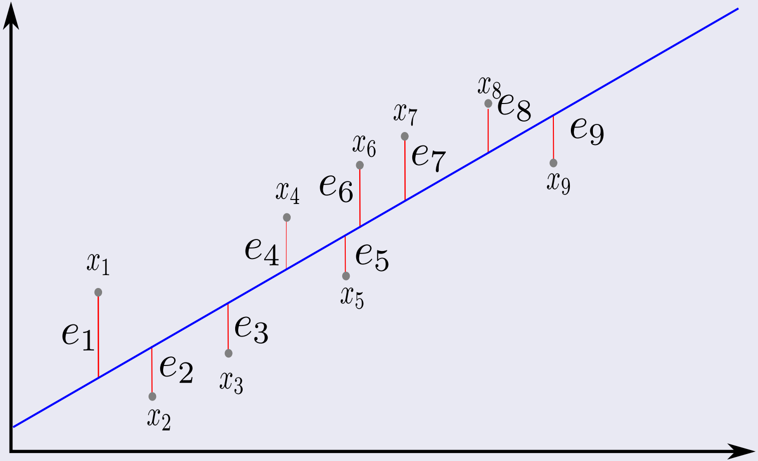
Here, we have multiple errors

What can we do?



Sum Over All the Errors

We can do the following

$$J(\boldsymbol{w}) = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} \left(y_i - g_{ideal}(\boldsymbol{x}_i)\right)^2 \quad (13)$$

Remark: This is know as the Least Squared Error cost function

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Generalizing

- The dimensionality of each sample (data point) is d.
- You can extend each vector sample to be $x^T = (1, x')$.

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We can use a trick

The following function

$$g_{ideal}(\boldsymbol{x}) = \begin{pmatrix} 1 & x_1 & x_2 & \dots & x_d \end{pmatrix} \begin{pmatrix} w_0 \\ w_2 \\ w_3 \\ \vdots \\ w_d \end{pmatrix} = \boldsymbol{x}^T \boldsymbol{w}$$

We can rewrite the error equation as

$$J(\boldsymbol{w}) = \sum_{i=1}^{N} \left(y_i - g_{ideal}(\boldsymbol{x}_i)\right)^2 = \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{w}\right)^2 \tag{14}$$

We can use a trick

The following function

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Furthermore

Then stacking all the possible estimations into the product Data Matrix and weight vector

$$\boldsymbol{X}\boldsymbol{w} = \begin{pmatrix} 1 & (\boldsymbol{x}_1)_1 & \cdots & (\boldsymbol{x}_1)_j & \cdots & (\boldsymbol{x}_1)_d \\ \vdots & & & \vdots & & \vdots \\ 1 & (\boldsymbol{x}_i)_1 & & (\boldsymbol{x}_i)_j & & (\boldsymbol{x}_i)_d \\ \vdots & & & \vdots & & \vdots \\ 1 & (\boldsymbol{x}_N)_1 & \cdots & (\boldsymbol{x}_N)_j & \cdots & (\boldsymbol{x}_N)_d \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_{d+1} \end{pmatrix}$$

Note about other representations

We could have $\boldsymbol{x}^T = (x_1, x_2, ..., x_d, 1)$ thus

$$\boldsymbol{X} = \begin{pmatrix} (\boldsymbol{x}_1)_1 & \cdots & (\boldsymbol{x}_1)_j & \cdots & (\boldsymbol{x}_1)_d & 1 \\ & & \vdots & & \vdots & \vdots \\ (\boldsymbol{x}_i)_1 & & (\boldsymbol{x}_i)_j & & (\boldsymbol{x}_i)_d & 1 \\ & & \vdots & & \vdots & \vdots \\ (\boldsymbol{x}_N)_1 & \cdots & (\boldsymbol{x}_N)_j & \cdots & (\boldsymbol{x}_N)_d & 1 \end{pmatrix} \quad (15)$$

Then, we have the following trick with $\boldsymbol{X}$

With the Data Matrix

$$\boldsymbol{X}w = \begin{pmatrix} \boldsymbol{x}_1^T\boldsymbol{w} \\ \boldsymbol{x}_2^T\boldsymbol{w} \\ \boldsymbol{x}_3^T\boldsymbol{w} \\ \vdots \\ \boldsymbol{x}_N^T\boldsymbol{w} \end{pmatrix} \quad (16)$$

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Therefore

We have that

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_4 \end{pmatrix} - \begin{pmatrix} \boldsymbol{x}_1^T \boldsymbol{w} \\ \boldsymbol{x}_2^T \boldsymbol{w} \\ \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} y_1 - \boldsymbol{x}_1^T \boldsymbol{w} \\ y_2 - \boldsymbol{x}_2^T \boldsymbol{w} \\ y_3 - \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ y_4 - \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix}$$

Then, we have the following equality

$$\begin{pmatrix} y_1 - \boldsymbol{x}_1^T \boldsymbol{w} & y_2 - \boldsymbol{x}_2^T \boldsymbol{w} & y_3 - \boldsymbol{x}_3^T \boldsymbol{w} & \cdots & y_4 - \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix} \begin{pmatrix} y_1 - \boldsymbol{x}_1^T \boldsymbol{w} \\ y_2 - \boldsymbol{x}_2^T \boldsymbol{w} \\ y_3 - \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ y_4 - \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix} = \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{w} \right)^2$$

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Therefore

We have that

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_4 \end{pmatrix} - \begin{pmatrix} \boldsymbol{x}_1^T \boldsymbol{w} \\ \boldsymbol{x}_2^T \boldsymbol{w} \\ \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} y_1 - \boldsymbol{x}_1^T \boldsymbol{w} \\ y_2 - \boldsymbol{x}_2^T \boldsymbol{w} \\ y_3 - \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ y_4 - \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix}$$

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Then, we have

The following equality

$$\sum_{i=1}^{N}\left(y_i - \boldsymbol{x}_i^T \boldsymbol{w}\right)^2 = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 \qquad (17)$$

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We can expand our quadratic formula!!!

Thus

$$(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) = \boldsymbol{y}^T\boldsymbol{y} - \boldsymbol{y}^T\boldsymbol{X}\boldsymbol{w} - \boldsymbol{w}^T\boldsymbol{X}^T y + \boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} \quad (18)$$

We can expand our quadratic formula!!!

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$$\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}\right)^{T}\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}\right)=\boldsymbol{y}^{T}\boldsymbol{y}-\boldsymbol{y}^{T}\boldsymbol{X}\boldsymbol{w}-\boldsymbol{w}^{T}\boldsymbol{X}^{T}y+\boldsymbol{w}^{T}\boldsymbol{X}^{T}\boldsymbol{X}\boldsymbol{w} \quad (18)$$

Now

- Derive with respect to $\boldsymbol{w}$
- Assume that $X^T X$ is invertible

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$$(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})^T(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})=\boldsymbol{y}^T\boldsymbol{y}-\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{w}-\boldsymbol{w}^T\boldsymbol{X}^Ty+\boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} \quad (18)$$

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Outline

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Some Basic Definitions

Transpose of a Matrix

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}^T = \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}$$

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Additionally

We have

Given A and B matrices:

- $(A+B)^T = A^T + B^T$
- $(AB)^T = B^T A^T$

Given vectors x, y and a matrix A such that you can multiply them:

- $x^T A y = \left[x^T A y\right]^T = y^T A^T x$ given that the transpose of a number is the number itself.

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Some Basic Definitions for

Derivative on Matrices

$$\frac{dA\boldsymbol{x}}{d\boldsymbol{x}} = \frac{d\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}{d\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}$$

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Therefore

We have

$$\frac{d\begin{pmatrix} a_{11}x_1+ & a_{12}x_2+ & a_{13}x_3 \\ a_{21}x_1+ & a_{22}x_2+ & a_{23}x_3 \\ a_{31}x_1+ & a_{32}x_2+ & a_{33}x_3 \end{pmatrix}}{d\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}} = \dots$$

$$\begin{pmatrix} \frac{d(a_{11}x_1+a_{12}x_2+a_{13}x_3)}{dx_1} & \frac{d(a_{11}x_1+a_{12}x_2+a_{13}x_3)}{dx_2} & \frac{d(a_{11}x_1+a_{12}x_2+a_{13}x_3)}{dx_3} \\ \frac{d(a_{21}x_1+a_{22}x_2+a_{23}x_3)}{dx_1} & \frac{d(a_{21}x_1+a_{22}x_2+a_{23}x_3)}{dx_2} & \frac{d(a_{21}x_1+a_{22}x_2+a_{23}x_3)}{dx_3} \\ \frac{d(a_{31}x_1+a_{32}x_2+a_{33}x_3)}{dx_1} & \frac{d(a_{31}x_1+a_{32}x_2+a_{33}x_3)}{dx_2} & \frac{d(a_{31}x_1+a_{32}x_2+a_{33}x_3)}{dx_3} \end{pmatrix} = \dots$$

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$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

Therefore

We have the following equivalences

$$\frac{d\boldsymbol{w}^T A \boldsymbol{w}}{d\boldsymbol{w}} = \boldsymbol{w}^T \left(A + A^T\right), \; \frac{d\boldsymbol{w}^T A}{d\boldsymbol{w}} = A^T \tag{19}$$

Now given that the transpose of a number is the number itself

$$\boldsymbol{y}^T \boldsymbol{X} \boldsymbol{w} = \left[\boldsymbol{y}^T \boldsymbol{X} \boldsymbol{w}\right]^T = \boldsymbol{w}^T \boldsymbol{X}^T \boldsymbol{y}$$

Therefore

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Now given that the transpose of a number is the number itself

$$\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{w} = \left[\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{w}\right]^T = \boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{y}$$

Then, when we derive by $\boldsymbol{w}$

We have then

$$\frac{d\left(\boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{w}^T\boldsymbol{X}^T y + \boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}\right)}{d\boldsymbol{w}} = -2\boldsymbol{y}^T\boldsymbol{X} + \boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X} + \left(\boldsymbol{X}^T\boldsymbol{X}\right)\right)$$

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$$= -2\boldsymbol{y}^T\boldsymbol{X} + 2\boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)$$

Making this equal to the zero row vector

$$-2y^T X + 2w^T\left(X^T X\right) = 0$$

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$$-2\boldsymbol{y}^T\boldsymbol{X}+2\boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)=0$$

We apply the transpose

$$\left[-2\boldsymbol{y}^T\boldsymbol{X}+2\boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)\right]^T=[0]^T$$

$$-2\boldsymbol{X}^T\boldsymbol{y}+2\left(\boldsymbol{X}^T\boldsymbol{X}\right)\boldsymbol{w}=0 \text{ (column vector)}$$

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$$\frac{d\left(\boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{w}^T\boldsymbol{X}^T y + \boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}\right)}{d\boldsymbol{w}} = -2\boldsymbol{y}^T\boldsymbol{X} + \boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X} + \left(\boldsymbol{X}^T\boldsymbol{X}\right)\right)$$

$$= -2\boldsymbol{y}^T\boldsymbol{X} + 2\boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)$$

Making this equal to the zero row vector

$$-2\boldsymbol{y}^T\boldsymbol{X} + 2\boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X}\right) = 0$$

We apply the transpose

$$\left[-2\boldsymbol{y}^T\boldsymbol{X} + 2\boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X}\right)\right]^T = [0]^T$$

$$-2\boldsymbol{X}^T\boldsymbol{y} + 2\left(\boldsymbol{X}^T\boldsymbol{X}\right)\boldsymbol{w} = 0 \text{ (column vector)}$$

Solving for $\boldsymbol{w}$

We have then

$$\boldsymbol{w} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{y} \tag{20}$$

Note: $\boldsymbol{X}^T \boldsymbol{X}$ is always positive semi-definite. If it is also invertible, it is positive definite.

Thus, How we get the discriminant function?

Any Ideas?

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The Final Discriminant Function

Very Simple!!!

$$g(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{w} = \boldsymbol{x}^T \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{y} \quad (21)$$

Pseudo-inverse of a Matrix

Definition

Suppose that $X \in \mathbb{R}^{m \times n}$ and $rank\,(X) = m$. We call the matrix

$$\boldsymbol{X}^{+} = \left(\boldsymbol{X}^{T}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{T}$$

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X^{+} inverts X on its image

- If $x \in image\,(X)$, then there is some $z \in \mathbb{R}^{n}$ such that $x = Xz$.
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- First a definition
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- Hence, $\boldsymbol{X}^{+}\boldsymbol{w} = \boldsymbol{X}^{+}\boldsymbol{X}\boldsymbol{v} = \left(\boldsymbol{X}^{T}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{T}\boldsymbol{X}\boldsymbol{v} = \boldsymbol{v}$

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Outline

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We have that

The Data Matrix

$$\boldsymbol{X} \in \mathbb{R}^{N \times (d+1)}$$

$Image\left(\boldsymbol{X}\right)$

$$Image\left(\boldsymbol{X}\right) = span\left\{\boldsymbol{X}_1^{col}, ..., \boldsymbol{X}_{d+1}^{col}\right\}$$

Note: Remember that the image of a matrix $\boldsymbol{X}$ is all the vectors $\boldsymbol{X}\boldsymbol{v} \in \mathbb{R}^N$ with $\boldsymbol{v} \in \mathbb{R}^{d+1}$

The Inputs

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We can now see where $\boldsymbol{y}$ is being projected

Basically $\boldsymbol{y}$, the list of real inputs is being proyected into

$$span\left\{\boldsymbol{X}_1^{col}, \boldsymbol{X}_2^{col}, ..., \boldsymbol{X}_{d+1}^{col}\right\} \tag{22}$$

by the projection operator $\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T$.

Outline

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Geometric Interpretation

We have

The image of the mapping:

$$h : \boldsymbol{w} \longmapsto \boldsymbol{X}\boldsymbol{w}$$

$$h : \mathbb{R}^{d+1} \longmapsto \mathbb{R}^{N}$$

is a linear subspace of $\mathbb{R}^N$.

How? Ideas

Think about this!!!

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As $\boldsymbol{w}$ can moves through all points in $\mathbb{R}^{d+1}$ when being generated

The function value $h(\boldsymbol{w}) = \boldsymbol{X}\boldsymbol{w}$ can move through all points in the image space:

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What about the optimality of $\boldsymbol{w}$?

We have a composition of functions that are convex

$$f\left(\boldsymbol{w}\right) = \boldsymbol{w}^T\boldsymbol{x}$$
$$g\left(t\right) = \left(y - t\right)$$
$$h\left(e\right) = \sum_{i=1}^{n} e^2$$

- Making the Least Squared Error a Convex function with a single minimum!!!

The derivative method produces a $\widehat{\boldsymbol{w}}$

- Such that $\widehat{\boldsymbol{w}}$ minimizes the distance $d\left(\boldsymbol{y}, image\left(\boldsymbol{X}\right)\right)$.

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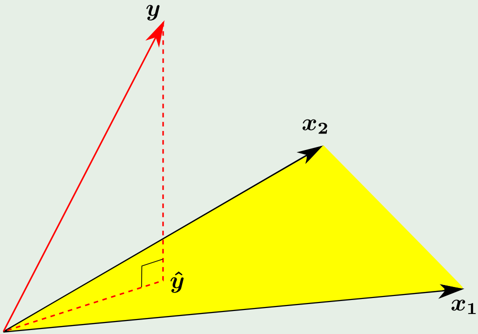
Geometrically

Given a $\boldsymbol{y}$, you obtain a projected $\widehat{\boldsymbol{y}}$ through the process $\boldsymbol{X}^T\boldsymbol{y}$



This Resolve Our Problem

With the Labels being chosen at the beginning

Question? Did you noticed the following?

We assume a similar number of elements in both classes

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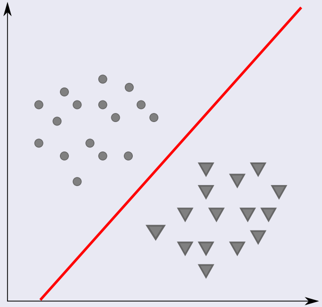

Outline

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Multi-Class Solution

What to do?

1. We might reduce the problem to $c-1$ two-class problems.
2. We might use $\frac{c(c-1)}{2}$ linear discriminants, one for every pair of classes.

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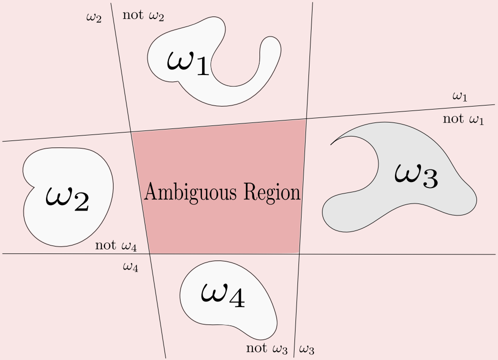

What to Do?

Define c linear discriminant functions

$$g_i\left(\boldsymbol{x}\right) = \boldsymbol{w}^T\boldsymbol{x} + w_{i0} \text{ for } i = 1, ..., c \tag{23}$$

This is known as a linear machine

Rule: if $g_k\left(\boldsymbol{x}\right) > g_j\left(\boldsymbol{x}\right)$ for all $j \neq k \Longrightarrow \boldsymbol{x} \in \omega_k$

- Decision Regions are Convex.

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Nice Properties (It can be proved!!!)

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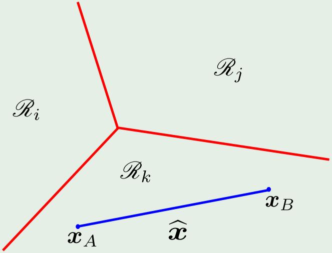

Actually quite simple

Given

$$y = \lambda x_A + (1 - \lambda) x_B$$

with $\lambda \in (0, 1)$.

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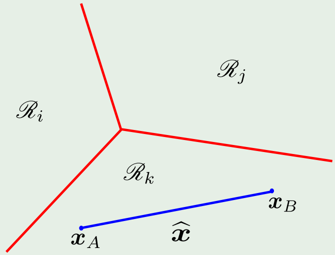

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For all $j \neq k$

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- y belongs to an area k defined by the rule!!!
- This area is **Convex** and **Singly Connected** because the definition of y.

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However!!!

No so nice properties!!!

- **It limits the power of classification for multi-objective function.**

How do we train this Linear Machine?

We know that each ω_k class is described by

$$g_k(\boldsymbol{x}) = \boldsymbol{w}_k^T \boldsymbol{x} + w_0 \text{ where } k = 1, ..., c$$

We then design a single machine

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\boldsymbol{W}^T = \begin{pmatrix} 1 & w_{11} & w_{12} & \cdots & w_{1d} \\ 1 & w_{21} & w_{22} & \cdots & w_{2d} \\ 1 & w_{31} & w_{32} & \cdots & w_{3d} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & w_{c1} & w_{c2} & \cdots & w_{cd} \end{pmatrix} \tag{25}
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What about the labels?

OK, we know how to do with 2 classes, What about many classes?

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Use a vector $\boldsymbol{t}_i$ with dimensionality c to identify each element at each class

We have then the following dataset

$$\{\boldsymbol{x}_i, \boldsymbol{t}_i\} \text{ for } i = 1, 2, ..., N$$

We build the following Matrix of Vectors

$$T = \begin{pmatrix} \boldsymbol{t}_1^T \\ \boldsymbol{t}_2^T \\ \vdots \\ \boldsymbol{t}_{N-1}^T \\ \boldsymbol{t}_N^T \end{pmatrix} \quad (26)$$

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Examples for the $\boldsymbol{t}_i$

Vectors like

$$x_i \neq 0, i \text{ Class} \rightarrow \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Another possible vector

$$x_i \neq -1, i \text{ Class} \rightarrow \begin{pmatrix} -1 \\ -1 \\ \vdots \\ -1 \\ 1 \\ -1 \\ \vdots \\ -1 \end{pmatrix}$$

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A Matrix containing all the required information

$$XW - T \tag{27}$$

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Remark: It is the vector result of multiplication of row i of $\boldsymbol{X}$ against $\boldsymbol{W}$ on $\boldsymbol{X}\boldsymbol{W}$.

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That is compared to the vector $\boldsymbol{t}_i^T$ on $\boldsymbol{T}$ by using the subtraction of vectors

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What do we want?

We want the quadratic error

$$\frac{1}{2}e_i^2$$

This specific quadratic errors are at the diagonal of the matrix

$$\left(\boldsymbol{XW}-\boldsymbol{T}\right)^T\left(\boldsymbol{XW}-\boldsymbol{T}\right)$$

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The trace allows to express the total error

$$J\left(\boldsymbol{W}\right) = \frac{1}{2} Trace\left\{\left(\boldsymbol{X}\boldsymbol{W} - \boldsymbol{T}\right)^T \left(\boldsymbol{X}\boldsymbol{W} - \boldsymbol{T}\right)\right\} \quad (31)$$

Thus, we have by the same derivative method

$$\boldsymbol{W} = \left(\boldsymbol{X}^T \boldsymbol{X}\right) \boldsymbol{X}^T \boldsymbol{T} = \boldsymbol{X}^{+} \boldsymbol{T} \quad (32)$$

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Thus, we obtain the discriminant

$$g(\boldsymbol{x}) = \boldsymbol{W}^T \boldsymbol{x} = \boldsymbol{T}^T \left(\boldsymbol{X}^+\right)^T \boldsymbol{x} \tag{33}$$

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Outline

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Let me show you the covariance matrix

We have in matrix notation

$$S = \frac{1}{N-1}\left(X - \mathbf{1}\overline{\boldsymbol{x}}^{T}\right)^{T}\left(X - \mathbf{1}\overline{\boldsymbol{x}}^{T}\right)$$

- It is the same dependency as the dependency between the features in the data observed after the featured have been centered by

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We can apply a similar analysis...

To obtain some of the possible cases that make $X^T X$ singular

A Classical One

- If there is a interdependence between features
  - Meaning some feature is an exact linear combination of the other features.
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When does this happen?

First

Number of features is equal or greater than the number of samples.

Second

Two or more features sum up to a constant

- For example, $x_2 - 5x_{10} = 0$

Third

Two features are identical or differ merely in mean or variance.

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Still

The least squares coefficients $\widehat{\boldsymbol{w}}$ are not uniquely defined.

- The fitted values $\widehat{\boldsymbol{y}} = \boldsymbol{X}\widehat{\boldsymbol{w}}$ are still the projection of $\boldsymbol{y}$ onto the column space of $\boldsymbol{X}$.

Additionally

Duplicate observations in a data set

It will lead the matrix toward singularity.

Cautionary Tale

When doing some sort of imputation of missing features it is always beneficial (from both statistical and mathematical view) to add some noise to the imputed data.

This can happen in the preprocessing phase

Be careful.

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The non-full-rank case occurs

- Most often when one or more qualitative inputs are coded in a redundant fashion.

How do we solve this?

- Re-encode or dropping redundant columns in X.

Most regression software packages

- They detect these redundancies and automatically implement some strategies for removing them.

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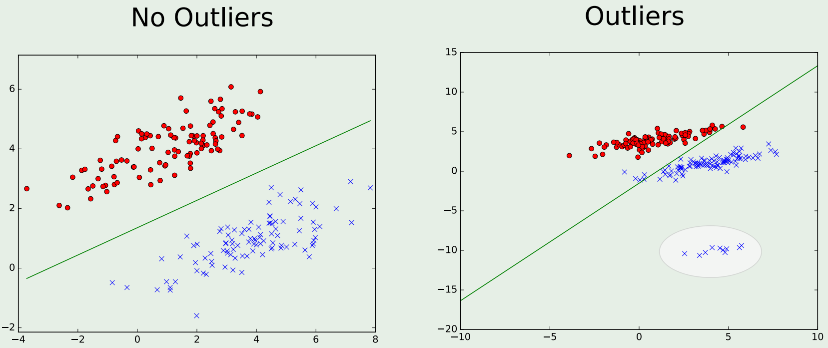
Issues with Least Squares

Problem with Outliers



Outline

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Problems with a High Number of Dimensions

In Many Modern Problems

- Many dimensions/features/predictors (possibly thousands).

- Possible some type of regularization

- Relevant dimensions might be averaged with irrelevant ones

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We will start using some statistics

We want to obtain sampling properties for $\widehat{\boldsymbol{w}}$

For this remember:

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

For this assume,

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Then, we have the variance-covariance matrix

We have

$$Var\left(\widehat{\boldsymbol{w}}\right) = Var\left[\left(\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{y}\right]$$

We have the following equivalence

$$Var\left(Ay\right) = AVar\left(y\right)A^{T}$$

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Something Notable

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Typically, we can use the following unbiased estimator

$$\widehat{\sigma}^2 = \frac{1}{N-d-1}\sum_{i=1}^{N}\left(y_i - \widehat{y}_i\right)$$

- Which is an unbiased estimator $E\left[\widehat{\sigma}^2\right] = \sigma^2$.

If we have the following relation

$$Y = E\left(Y|X_1, X_2, ..., X_d\right) + \epsilon$$

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$$\begin{aligned} H_0 &: \beta_j = 0 \\ H_1 &: \beta_j \neq 0 \end{aligned}$$

To test for Hypothesis 0, we get the following $z-$score

$$z_j = \frac{\widehat{\beta}_j - \beta_j}{\widehat{\sigma}\sqrt{v_j}} = \frac{\widehat{\beta}_j}{\widehat{\sigma}\sqrt{v_j}} \text{ with } v_j \text{ the } j^{th} \text{ diagonal element at } \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}$$

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$z_j \sim t_{N-d-1}$ a t-student distribution

- Therefore, a large(absolute) value of z_j will lead to rejection of the Null Hypothesis

- Accept H_0 remove the feature
- Reject H_0 keep the feature

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Outline

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Definition

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Imagine the following in $\mathbb{R}^3$

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They span a subspace for those column vectors in $\mathbb{R}^3$

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$$span \left\{ \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix}, \begin{pmatrix} a_{12} \\ a_{22} \\ a_{32} \end{pmatrix}, \begin{pmatrix} a_{13} \\ a_{23} \\ a_{33} \end{pmatrix} \right\}$$

Relation with the Rank

If a matrix is singular

Its Rank is less than 3, i.e :

1. The subspace is squashed into a plane.
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Remember

That, we have

$$\boldsymbol{v} = \lambda_1 \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} + \lambda_2 \begin{pmatrix} a_{12} \\ a_{22} \\ a_{32} \end{pmatrix} + \lambda_3 \begin{pmatrix} a_{13} \\ a_{23} \\ a_{33} \end{pmatrix}$$

Thus, if for example, the matrix projects into a plane

$$\begin{aligned}\boldsymbol{v} =& \lambda_1 \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} + \lambda_2 \left[\alpha_1 \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} + \alpha_2 \begin{pmatrix} a_{13} \\ a_{23} \\ a_{33} \end{pmatrix} \right] + \lambda_3 \begin{pmatrix} a_{13} \\ a_{23} \\ a_{33} \end{pmatrix} \\ =& c_1 \begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} + c_2 \begin{pmatrix} a_{13} \\ a_{23} \\ a_{33} \end{pmatrix} \text{ with } c_1 = \lambda_1 + \alpha_1 \lambda_2, c_2 = \alpha_2 \lambda_2 + \lambda_3\end{aligned}$$

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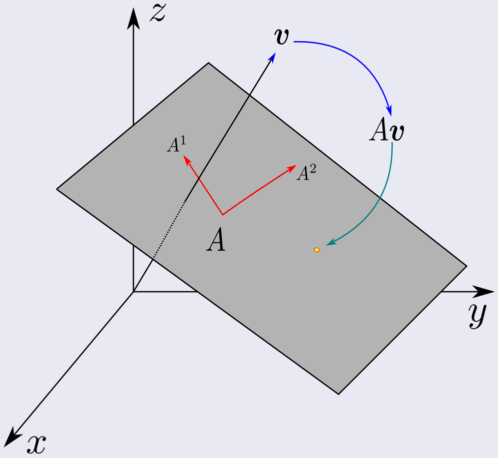
For Example

We have a squashing into a plane



Computational Intuition

First Intuition

A singular matrix maps an entire linear subspace into a single point.

Second Intuitions

If a matrix maps points far away from each other to points very close to each other, it almost behaves like a singular matrix.

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Mapping is related to the eigenvalues!!!

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All this comes from the following statement

A positive semi-definite matrix A is singular $\iff$ smallest eigenvalue is 0

Consequence for Statistics

If a statistical prediction involves the inverse of an almost-singular matrix, the predictions become unreliable (high variance).

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What can be done?

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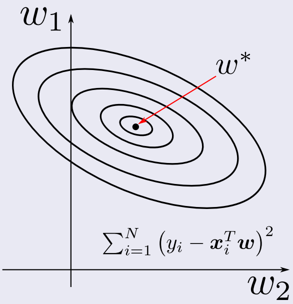

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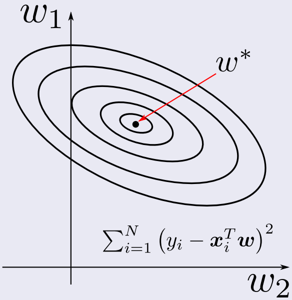

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IDEAS?

We want to avoid the problem of an eigenvalue to become zero!!!

Thus, we can do the following given that $X^T X$ is positive definite

Assume that $\xi_1, \xi_2, ..., \xi_{d+1}$ are eigenvectors of $\boldsymbol{X}^T\boldsymbol{X}$ with eigenvalues $\lambda_1, \lambda_2, ..., \lambda_{d+1}$

We have

$$\left(\boldsymbol{X}^T\boldsymbol{X}\right)\xi_i = \lambda_i \xi_i \text{ for all } i = 1, ..., d+1 \quad (34)$$

Given that $\boldsymbol{X}^T\boldsymbol{X}$ is singular, some λ_i is equal to 0.

Very Simple, add a convenient λ

$$\left(\boldsymbol{X}^T\boldsymbol{X} + \lambda I\right)\xi_i = (\lambda_i + \lambda)\,\xi_i \quad (35)$$

i.e. $\lambda_i + \lambda$ is an eigenvalue for $\left(\boldsymbol{X}^T\boldsymbol{X} + \lambda I\right)$.

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We modify it by adding en extra parameter

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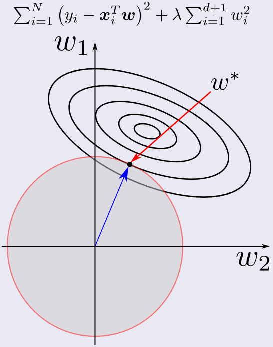

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Exercises

Duda and Hart

Chapter 5

- 1, 3, 4, 7, 13, 17

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Chapter 4

- 4.1, 4.4, 4.7,

Hastie-Tibishirani

Chapter 3 - Problems

- Ex 3.5
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Theodoridis

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