The Data Science Cycle

Unsupervised Learning - Clustering

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September 21, 2016

Outline

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Outline

What is it?

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

Here, we have an hyperplane as a model:

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

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

We have the following function:

$$g(\boldsymbol{x}) = w_1 x_1 + w_2 x_2 + w_0 \tag{2}$$

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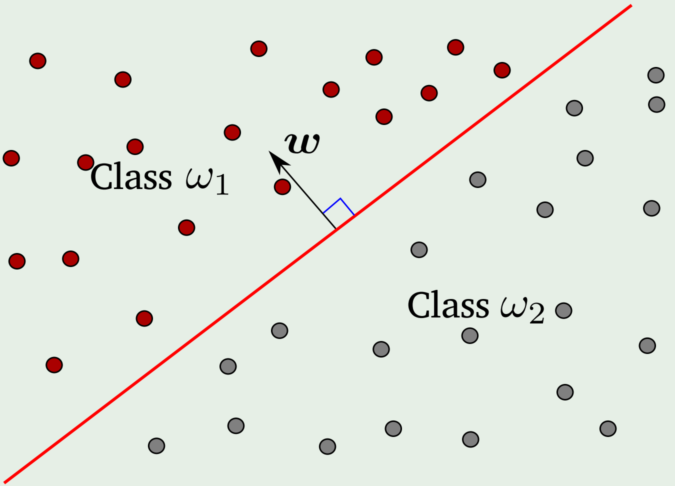
Splitting The Space $\mathbb{R}^2$

Using a simple straight line



Outline

Defining a 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

Given 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

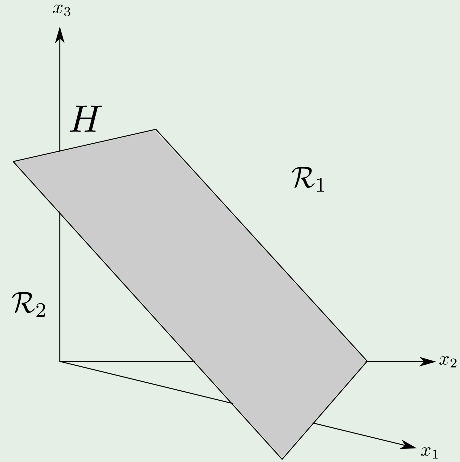
Thus

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

Remark: Any vector in the hyperplane is perpendicular to $\boldsymbol{w}^T$ i.e. $\boldsymbol{w}^T$ is normal to the hyperplane.

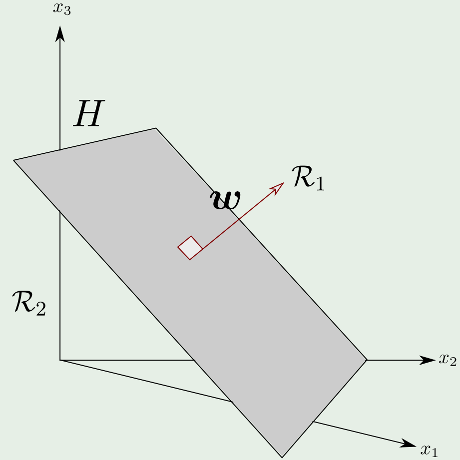
Therefore

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



Some Properties of the Hyperplane

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



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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
  - Negative, if x is in the negative side

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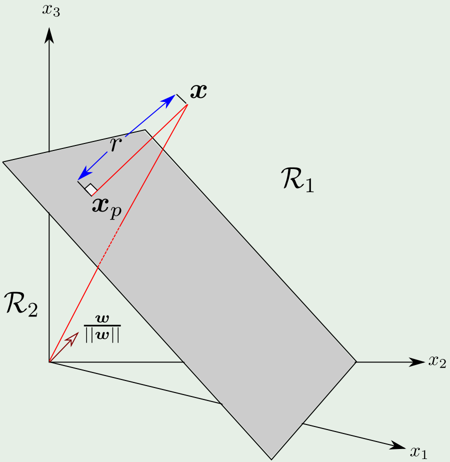

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In particular

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 $\boldsymbol{w}^T\boldsymbol{x}$ and hyperplane passes through the origin.

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In addition...

If we do the following

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

By making

$$x_0 = 1 \text{ and } \boldsymbol{y} = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{pmatrix} = \begin{pmatrix} 1 \\ \boldsymbol{x} \end{pmatrix}$$

Where

$\boldsymbol{y}$ is called an augmented feature vector.

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We have the augmented weight vector

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Initial Setup

Important

We get away from our initial normalization of the samples!!!

Now, we are going to use the method know as

Minimum Squared Error

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A Simple Solution For Our Quandary

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Assume true function f is given by

$$y_{noise} = g_{noise}\left(\boldsymbol{x}\right) = \boldsymbol{w}^T\boldsymbol{x} + w_0 + \epsilon \tag{8}$$

Where the ϵ

It has a $\epsilon \sim N\left(\mu, \sigma^2\right)$

Thus, we can do the following

$$y_{noise} = g_{noise}\left(\boldsymbol{x}\right) = g_{ideal}\left(\boldsymbol{x}\right) + \epsilon \tag{9}$$

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What to do?

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Graphically

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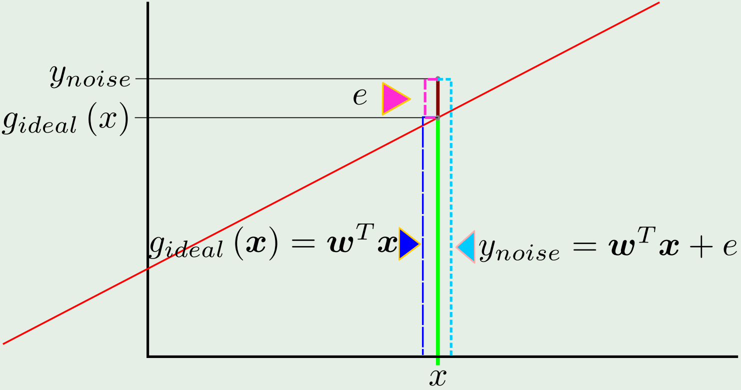

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Sum Over All Errors

We can do the following

$$J(\boldsymbol{w}) = \sum_{i=1}^{N} \epsilon_i^2 = \sum_{i=1}^{N} (y_i - g_{ideal}(\boldsymbol{x}))^2 \tag{11}$$

Remark: Know as least squares (Fitting the vertical offset!!!)

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Generalize

If

- The dimensionality of each sample (data point) is d,
- You can extend each vector sample to be $\boldsymbol{x}^T = (1, \boldsymbol{x}')$,
- We have:

$$\sum_{i=1}^{N} \left(y_i - \boldsymbol{x}^T \boldsymbol{w}\right)^2 = (\boldsymbol{y} - X\boldsymbol{w})^T (\boldsymbol{y} - X\boldsymbol{w}) = \|\boldsymbol{y} - X\boldsymbol{w}\|_2^2 \tag{12}$$

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What is $\boldsymbol{X}$

It is the Data Matrix

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\boldsymbol{X} = \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} \tag{13}
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We know the following

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\frac{dx^T A x}{dx} = Ax + A^T x, \quad \frac{dAx}{dx} = A \tag{14}
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Note about other representations

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

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

We can expand our quadratic formula!!!

Thus

$$(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})^{T}(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})=\boldsymbol{y}^{T}\boldsymbol{y}-\boldsymbol{w}^{T}\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{y}-\boldsymbol{y}^{T}\boldsymbol{X}\boldsymbol{w}+\boldsymbol{w}^{T}\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{X}\boldsymbol{w} \quad (16)$$

Making Possible to have by deriving with respect to w and assuming that $X^{T}X$ is invertible

$$\hat{w}=\left(X^{T}X\right)^{-1}X^{T}y \quad (17)$$

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The Final Discriminant Function

Very Simple!!!

$$g(\boldsymbol{x}) = \boldsymbol{x}^T \hat{\boldsymbol{w}} = \boldsymbol{x}^T \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{y} \quad (18)$$

Pseudo-inverse of a Matrix

Definition

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

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

the pseudo inverse of A.

Reason

A^{+} inverts A on its image

What?

If $w \in image\,(A)$, then there is some $v \in \mathbb{R}^{n}$ such that $w = Av$. Hence:

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Geometric Interpretation

We have

1. The image of the mapping $\boldsymbol{w}$ to $\boldsymbol{X}\boldsymbol{w}$ is a linear subspace of $\mathbb{R}^N$.
2. As $\boldsymbol{w}$ runs through all points $\mathbb{R}^{d+1}$, the function value $\boldsymbol{X}\boldsymbol{w}$ runs through all points in the image space $image\left(\boldsymbol{X}\right) = span\left\{\boldsymbol{X}_{\boldsymbol{1}}^{\boldsymbol{col}}, ..., \boldsymbol{X}_{\boldsymbol{d+1}}^{\boldsymbol{col}}\right\}$.
3. Each $\boldsymbol{w}$ defines one point $\boldsymbol{X}\boldsymbol{w} = \sum_{j=0}^{d} w_j \boldsymbol{X}_j^{col}$.
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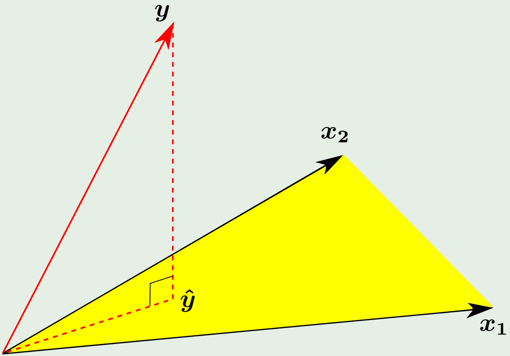
Geometrically

Ahhhh!!!



Outline

DataLab
Data Science Community

Issues with Least Squares

Robustness

1. Least squares works only if $\boldsymbol{X}$ has full column rank, i.e. if $\boldsymbol{X}^T\boldsymbol{X}$ is invertible.
2. If X^TX almost not invertible, least squares is numerically unstable.
    1. Statistical consequence: High variance of predictions.

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Problem with Outliers