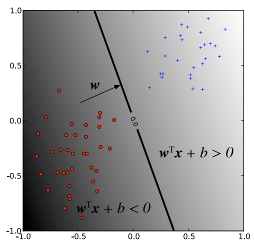
Linear models: the perceptron and closest centroid algorithms

Chapter 1, 7



Preliminaries

Definition: The Euclidean dot product between two vectors is the expression

$$\mathbf{w}^T\mathbf{x} = \sum_{i=1}^{d} w_i x_i$$

The dot product is also referred to as inner product or scalar product.

It is sometimes denoted as $\mathbf{w} \cdot \mathbf{x}$

(hence the name dot product).

Geometric interpretation. The dot product between two unit vectors is the cosine of the angle between them.

The dot product between a vector and a unit vector is the length of its projection in that direction.

Labeled data

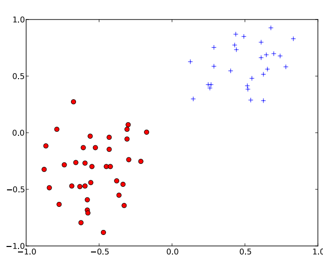
A labeled dataset:

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$$

Where $\mathbf{x}_i \in \mathbb{R}^d$ are d-dimensional vectors

The labels:

are discrete for classification problems (e.g. +1, -1) for binary classification



Labeled data

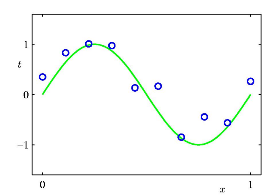
A labeled dataset:

$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$$

Where $\mathbf{x}_i \in \mathbb{R}^d$ are d-dimensional vectors

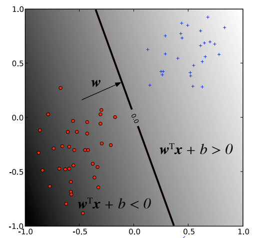
The labels:

are continuous values for a regression problem

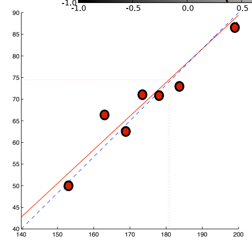


Linear models

Linear models for classification



Linear models for regression



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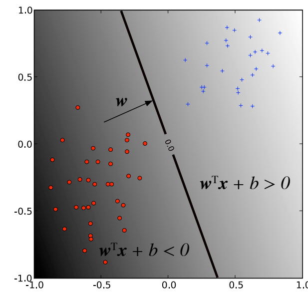
Linear models for classification



Discriminant/scoring function: $f(\mathbf{x}) = \underbrace{\mathbf{w}}_{\text{weight vector}} \cdot \mathbf{x} + \underbrace{b}_{\text{bias}}$

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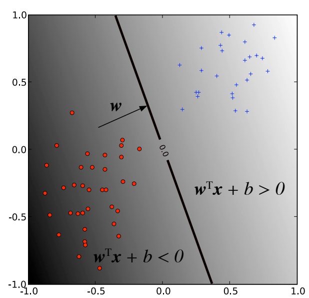
Linear models for classification



Decision boundary:

all x such that $f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + b = 0$

For linear models the the decision boundary is a line in 2-d, a plane in 3-d and a hyperplane in higher dimensions

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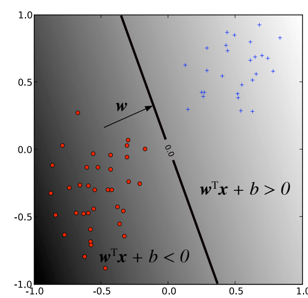
Linear models for classification



Using the discriminant to make a prediction: $\hat{y} = \text{sign}(\mathbf{w} \cdot \mathbf{x} + b)$

the sign function equals 1 when its argument is positive and -1 otherwise

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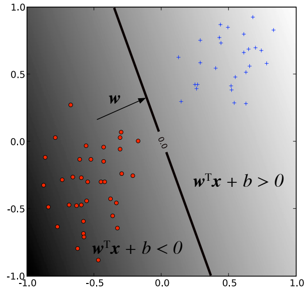
Linear models for classification



Decision boundary:
all x such that $f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + b = 0$

What can you say about the decision boundary when b = 0?

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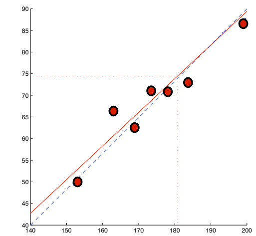
Linear models for regression

When using a linear model for regression the scoring function is the prediction:

$$\hat{y} = \mathbf{w} \cdot \mathbf{x} + b$$



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Why linear?

- It's a good baseline: always start simple
- Linear models are stable
- Linear models are less likely to overfit the training data because they have relatively less parameters. Can sometimes underfit. Often all you need when the data is high dimensional.
- Lots of scalable algorithms

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Closest centroid classifier

Define:

$$\boldsymbol{\mu}^{(+)} = \frac{1}{Pos} \sum_{\{i|y_i=1\}} \mathbf{x}_i \qquad \boldsymbol{\mu}^{(-)} = \frac{1}{Neg} \sum_{\{i|y_i=-1\}} \mathbf{x}_i$$

where Pos/Neg is the number of positive/negative examples.
This is the center of mass of the positive/negative examples.

Classify an input x according to which center of mass it is closest to.

Let's express this as a linear classifier!

See page 21-22 in the textbook

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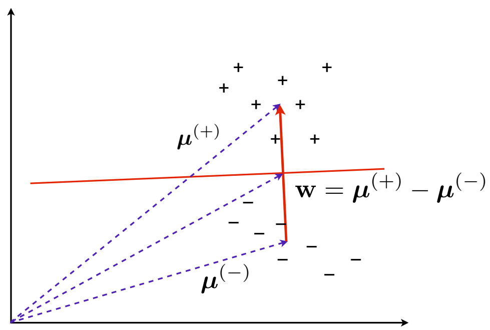
Closest centroid classifier



Our hyperplane is going be perpendicular to the vector that connects the two centers of mass. Therefore:

$$\mathbf{w} = \mu^{(+)} - \mu^{(-)}$$

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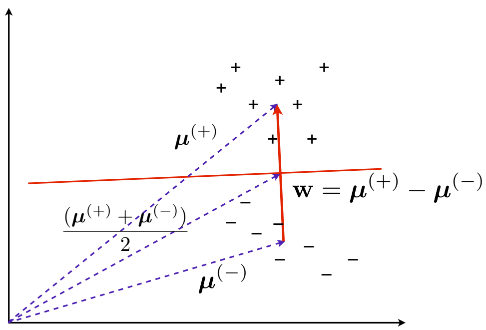
Closest centroid classifier



To find the bias term we use the fact that the midpoint between the means is on the hyperplane, i.e.

$$\mathbf{w} \cdot \frac{(\mu^{(+)} + \mu^{(-)})}{2} + b = 0$$

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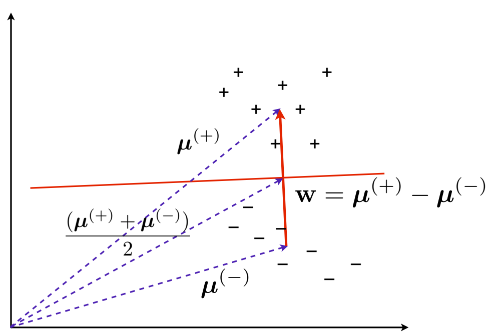
Closest centroid classifier



With a little algebra:
$$b = -\frac{1}{2}(\mu^{(+)} - \mu^{(-)})(\mu^{(+)} + \mu^{(-)})$$
$$= -\frac{1}{2}(||\mu^{(+)}||^2 - ||\mu^{(-)}||^2)$$

The norm of a vector:
$$||\mathbf{x}||^2 = \mathbf{x} \cdot \mathbf{x}$$

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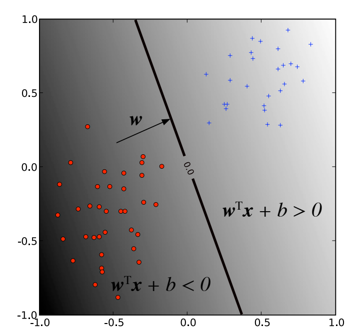
Linearly separable data

Linearly separable data: there exists a linear decision boundary separating the classes.

Example:



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The bias and homogeneous coordinates

In some cases we will use algorithms that learn a discriminant function without a bias term. This does not reduce the expressivity of the model because we can obtain a bias using the following trick:

Add another dimension x_0 to each input and set it to 1.

Learn a weight vector of dimension d+1 in this extended space, and interpret w_0 as the bias term. With the notation

$$\mathbf{w} = (w_1, \ldots, w_d) \qquad \tilde{\mathbf{w}} = (w_0, w_1, \ldots, w_d)$$

$$\tilde{\mathbf{x}} = (1, x_1, \ldots, x_d)$$

We have that:

$$\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}} = w_0 + \mathbf{w} \cdot \mathbf{x}$$

See page 4 in the book

The perceptron algorithm

Idea: iterate over the training examples, and update the weight vector w such that $\mathbf{x}_i$ is more likely to be correctly classified.

Let's assume that $\mathbf{x}_i$ is misclassified, and is a positive example i.e.

$$\mathbf{w} \cdot \mathbf{x}_i < 0$$

Note: we're learning a classifier without a bias term

We would like to update **w** to **w'** such that

$$\mathbf{w}' \cdot \mathbf{x}_i > \mathbf{w} \cdot \mathbf{x}_i$$

This can be achieved by choosing

$$\mathbf{w}' = \mathbf{w} + \eta \mathbf{x}_i$$

Where $0 < \eta \leq 1$ is the learning rate

Section 7.2 in the book

The perceptron algorithm

If $\mathbf{x}_i$ is a negative example, the update needs to be opposite.

Overall, we can summarize the two cases as:

$$\mathbf{w}' = \mathbf{w} + \eta y_i \mathbf{x}_i$$

```
Input:  labeled data D in homogeneous coordinates
Output:  weight vector w

w = 0
converged = false
while not converged :
    converged = true
    for i in 1,…,|D| :
        if xi is misclassified update w and set
            converged=false
```


The perceptron algorithm

The algorithm makes sense, but let's try to derive in a more principled way.

The algorithm is trying to find a vector **w** that separates positive from negative examples.

We can express that as:

$$y_i \mathbf{w}^{\mathsf{T}} \mathbf{x}_i > 0, \quad i = 1, \ldots, n$$

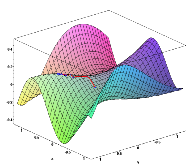
For a given weight vector **w** the degree to which this does not hold can be expressed as:

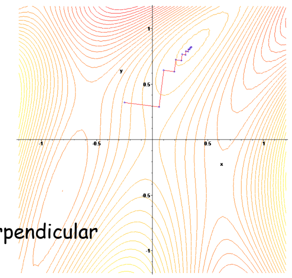
$$E(\mathbf{w}) = - \sum_{i:\ \mathbf{x}_i \text{ is misclassified}} y_i \mathbf{w}^{\mathsf{T}} \mathbf{x}_i$$

We want to find **w** that minimizes or maximizes this criterion?

Digression: gradient descent

Given a function E(**w**), the gradient is the direction of steepest ascent
Therefore to minimize E(**w**), take a step in the direction of the negative of the gradient





Notice that the gradient is perpendicular to contours of equal E(**w**)

Images from http://en.wikipedia.org/wiki/Gradient_descent

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Gradient descent

We can now express gradient descent as:

$$\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla E(\mathbf{w})$$
$$\mathbf{w}(t) - \eta \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$$

where
$$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = \left(\frac{\partial E(\mathbf{w})}{\partial w_1}, \ldots, \frac{\partial E(\mathbf{w})}{\partial w_d} \right)^{\mathsf{T}}$$

And **w**(t) is the weight vector at iteration t

The constant η is called the step size (learning rate when used in the context of machine learning).

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The perceptron algorithm

Let's apply gradient descent to the perceptron criterion:

$$E(\mathbf{w}) = - \sum_{i:\ \mathbf{x}_i \text{ is misclassified}} y_i \mathbf{w}^{\mathsf{T}} \mathbf{x}_i$$

$$\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} = - \sum_{i:\ \mathbf{x}_i \text{ is misclassified}} y_i \mathbf{x}_i$$

$$\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$$
$$= \mathbf{w}(t) + \eta \sum_{i:\ \mathbf{x}_i \text{ is misclassified}} y_i \mathbf{x}_i$$

Which is exactly the perceptron algorithm!

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The perceptron algorithm

The algorithm is guaranteed to converge if the data is linearly separable, and does not converge otherwise.

Issues with the algorithm:

- The algorithm chooses an arbitrary hyperplane that separates the two classes. It may not be the best one from the learning perspective.
- Does not converge if the data is not separable (can halt after a fixed number of iterations).

There are variants of the algorithm that address these issues (to some extent).

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Perceptron for regression

Replace the update equation with:

$$\mathbf{w}' = \mathbf{w} + \eta(y_i - \hat{y}_i)^2\mathbf{x}_i$$

This is not likely to converge so the algorithm is run for a fixed number of training epochs

Training epoch – one complete run through the training data