

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).

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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

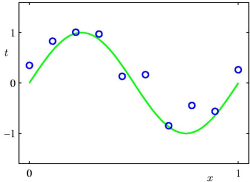
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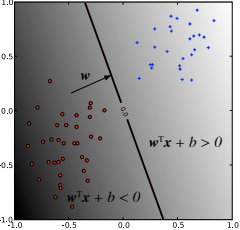
are continuous values for a regression problem



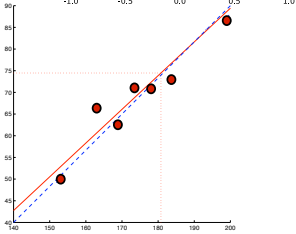
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Linear models

Linear models for classification

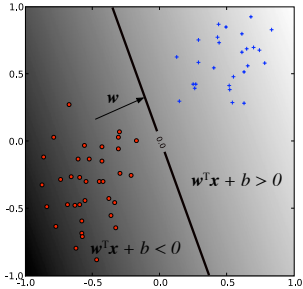


Linear models for regression



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Linear models for classification

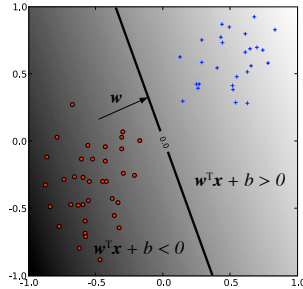


Discriminant/scoring function: $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$

↑ weight vector ↑ bias

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Linear models for classification



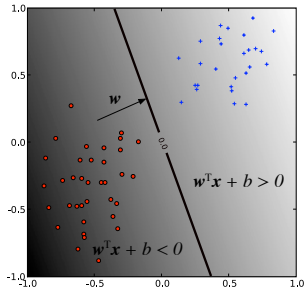
Decision boundary:

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

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

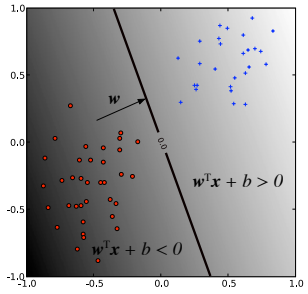


Using the discriminant to make a prediction: $\hat{y} = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$

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

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Linear models for classification



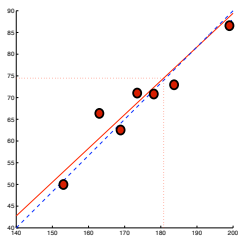
Decision boundary:
all \mathbf{x} such that $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = 0$

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:

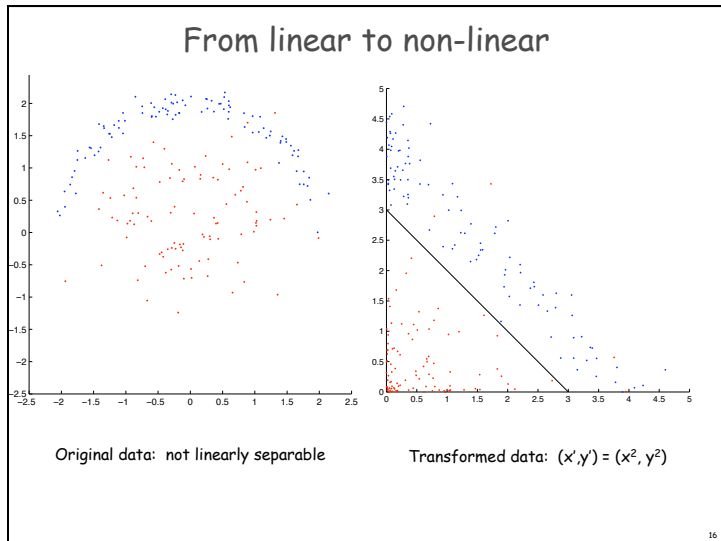
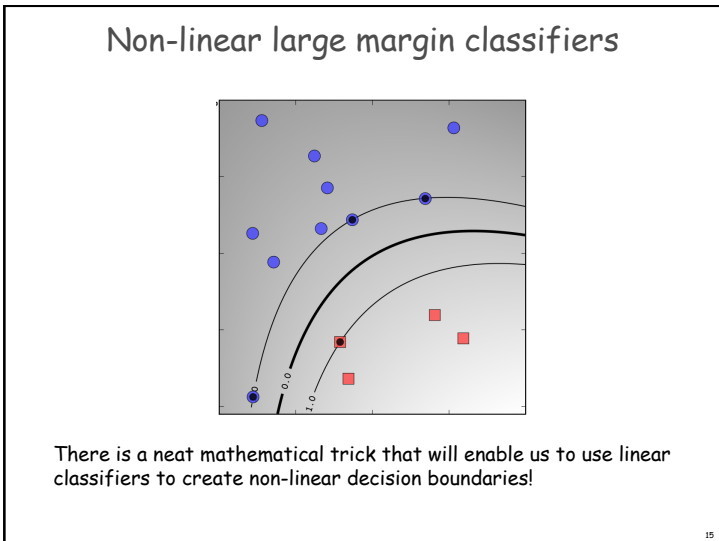
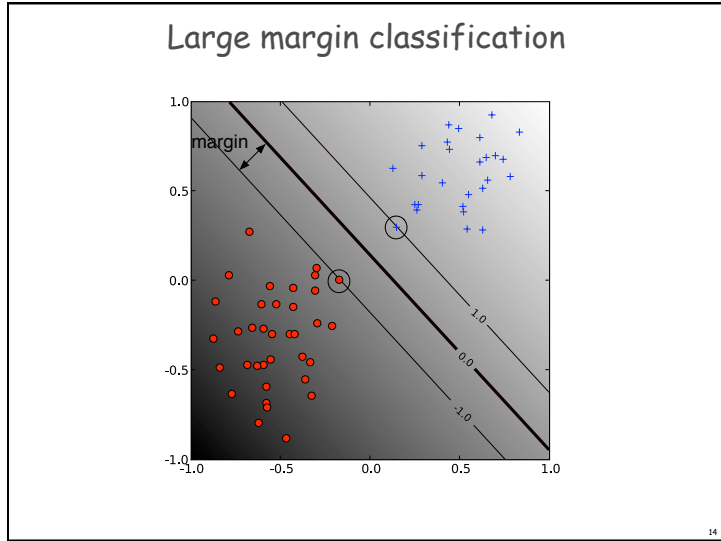
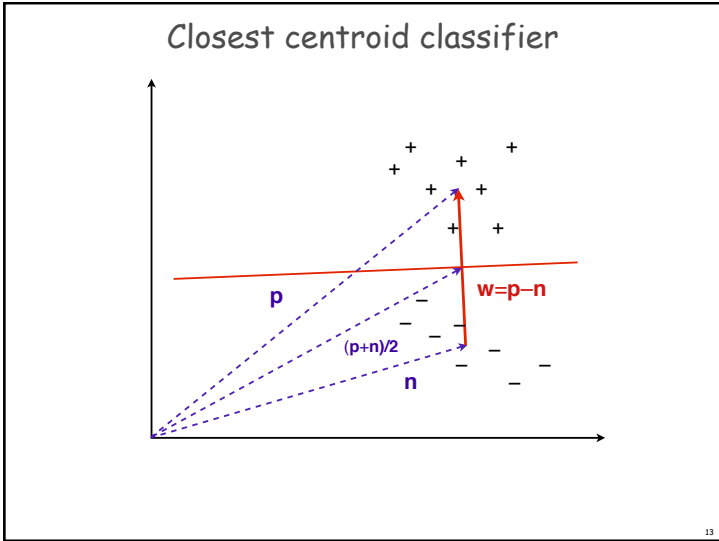
$$\hat{y} = \mathbf{w}^T \mathbf{x} + b$$


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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:

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

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

Classify an input \mathbf{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

Closest centroid classifier

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

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

Closest centroid classifier

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

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

Closest centroid classifier

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

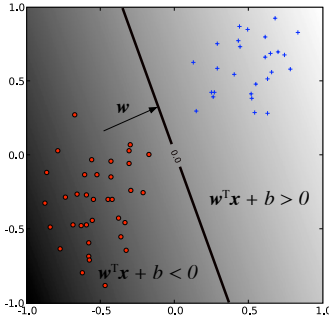
The norm of a vector: $\|\mathbf{x}\|^2 = \mathbf{x} \cdot \mathbf{x}$

$$= -\frac{1}{2}(\|\mu^{(+)}\|^2 - \|\mu^{(-)}\|^2)$$

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

$$\mathbf{w} = (w_1, \dots, w_d) \quad \tilde{\mathbf{w}} = (w_0, w_1, \dots, w_d)$$

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

We have that:

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

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See page 4 in the book

The perceptron algorithm (Rosenblatt, 1957)

Idea: iterate over the training examples, and update the weight vector w in a way that would make x_i more likely to be correctly classified.

Let's assume that 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

Rosenblatt, Frank (1957), The Perceptron--a perceiving and recognizing automaton. Report 85-460-1, Cornell Aeronautical Laboratory.

Section 7.2 in the book

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The perceptron algorithm

If 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 \mathbf{w}

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 $\mathbf{w} = 0$ 
converged = false
while not converged :
    converged = true
    for i in 1,..., |D| :
        if  $\mathbf{x}_i$  is misclassified update  $\mathbf{w}$  and set
            converged=false
                
```

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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:

$$y_i w^T x_i > 0, \quad i = 1, \dots, n$$

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

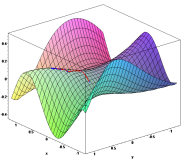
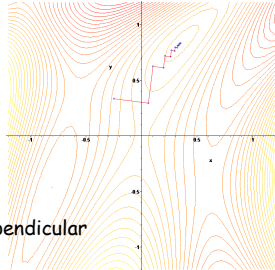
$$E(w) = - \sum_{i: x_i \text{ is misclassified}} y_i w^T x_i$$

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

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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 $E(w)$

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Gradient descent

We can now express gradient descent as:

$$w(t+1) = w(t) - \eta \nabla E(w)$$

$$w(t) - \eta \frac{\partial E(w)}{\partial w}$$

where

$$\frac{\partial E(w)}{\partial w} = \left(\frac{\partial E(w)}{\partial w_1}, \dots, \frac{\partial E(w)}{\partial w_d} \right)^T$$

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:

$$E(w) = - \sum_{i: x_i \text{ is misclassified}} y_i w^T x_i$$

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

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

$$= w(t) + \eta \sum_{i: x_i \text{ is misclassified}} y_i x_i$$

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

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