

# Artificial Intelligence

## EDAF70

### Lecture 8: Machine Learning (II)

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# Linear Classifiers

Similar to decision trees, discriminant analysis provides another set of techniques to learn classifiers from data sets.

This time, the objects will be represented by a vector of numerical parameters, often called the **features**.

Linear classification methods operate in an  $n$ -dimensional space with a vector space equal to the number of features.

Linear classifiers include:

- ① Perceptron
- ② Logistic regression
- ③ Support vector machines
- ④ Neural networks



# Problem Formulation

We can formulate the problem as finding lines automatically to:

- 1 Fit a data set (regression). The output is a real continuous variable.
- 2 Separate classes inside a data set (discriminant analysis, classification). The output is a discrete set of symbols, the classes, for instance  $\{0, 1\}$  or  $\{\text{negative}, \text{positive}\}$ .

Here, we will consider the binary case only with two classes. Multiclass classification is a generalization of it.

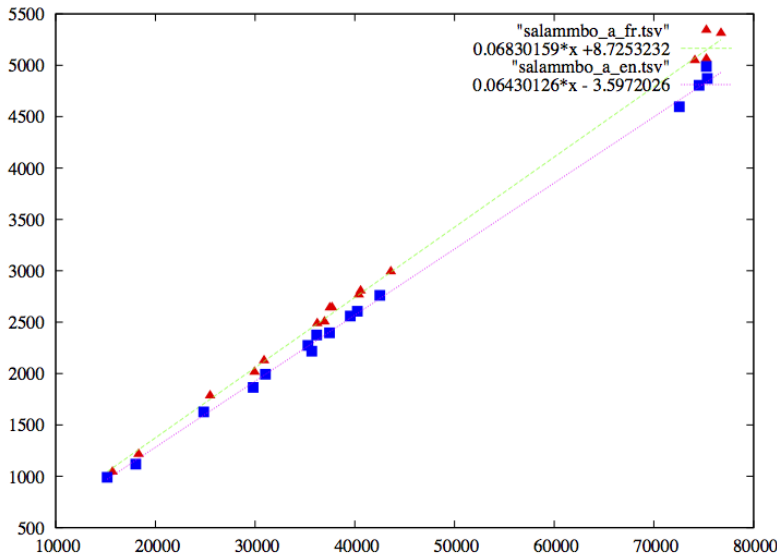


# Linear Regression: Letter Frequencies in *Salammbô*

| Chapter    | French       |        | English      |        |
|------------|--------------|--------|--------------|--------|
|            | # characters | # A    | # characters | # A    |
| Chapter 1  | 36,961       | 2,503  | 35,680       | 2,217  |
| Chapter 2  | 43,621       | 2,992  | 42,514       | 2,761  |
| Chapter 3  | 15,694       | 1,042  | 15,162       | 990    |
| Chapter 4  | 36,231       | 2,487  | 35,298       | 2,274  |
| Chapter 5  | 29,945       | 2,014  | 29,800       | 1,865  |
| Chapter 6  | 40,588       | 2,805  | 40,255       | 2,606  |
| Chapter 7  | 75,255       | 5,062  | 74,532       | 4,805  |
| Chapter 8  | 37,709       | 2,643  | 37,464       | 2,396  |
| Chapter 9  | 30,899       | 2,126  | 31,030       | 1,993  |
| Chapter 10 | 25,486       | 1,784  | 24,843       | 1,627  |
| Chapter 11 | 37,497       | 2,641  | 36,172       | 2,375  |
| Chapter 12 | 40,398       | 2,766  | 39,552       | 2,560  |
| Chapter 13 | 74,105       | 5,047  | 72,545       | 4,597  |
| Chapter 14 | 76,725       | 5,312  | 75,352       | 4,871  |
| Chapter 15 | 18,317       | 1,215  | 18,031       | 1,119  |
| Total      | 619,431      | 42,439 | 608,230      | 39,056 |



# Fitting the Data



# Fitting Equations

In a two-dimensional space, the straight line fitting the points is given by:

$$\hat{y} = mx + b,$$

Minimize the loss between:

- The set of  $q$  observations:  $\{(x_i, y_i)\}_{i=1}^q$  and
- A perfect linear alignment:  $\{(x_i, f(x_i))\}_{i=1}^q$ , where  $f(x_i) = mx_i + b$ .

The loss is traditionally modeled by the quadratic error (Legendre 1805):

$$L_2 = \sum_{\text{Set of points}} (y - \hat{y})^2.$$

For  $q$  points  $(x_i, y_i)$ :

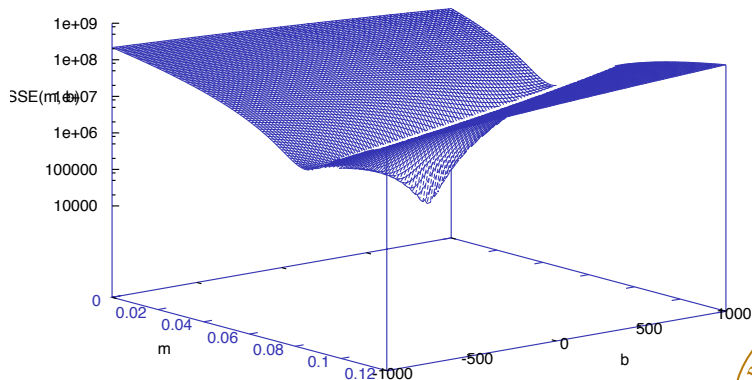
$$\text{Loss}(b, m) = \sum_{i=1}^q (y_i - (mx_i + b))^2$$

The objective of regression is to find the weights that minimize the loss



# Visualizing the Loss

SSE(x,y) —



# Minimizing the Loss

The loss function is convex and has a unique minimum.

The loss reaches a minimum when the partial derivatives are zero:

$$\begin{aligned}\frac{\partial \text{Loss}}{\partial m} &= \sum_{i=1}^q \frac{\partial}{\partial m} (y_i - (mx_i + b))^2 = -2 \sum_{i=1}^q x_i (y_i - (mx_i + b)) = 0 \\ \frac{\partial \text{Loss}}{\partial b} &= \sum_{i=1}^q \frac{\partial}{\partial b} (y_i - (mx_i + b))^2 = -2 \sum_{i=1}^q (y_i - (mx_i + b)) = 0\end{aligned}$$





# Fitting Equations (II)

This yields:

$$\begin{aligned} b &= \bar{y} - m\bar{x} \\ \sum_{i=1}^N x_i y_i - m \sum_{i=1}^q x_i^2 - q b \bar{x} &= \sum_{i=1}^q x_i y_i - m \sum_{i=1}^q x_i^2 - q \bar{x} (\bar{y} - m\bar{x}) = 0 \end{aligned}$$

$$m = \frac{\sum_{i=1}^q x_i y_i - q \bar{x} \bar{y}}{\sum_{i=1}^q x_i^2 - q \bar{x}^2} \quad \text{and} \quad b = \bar{y} - m\bar{x},$$

with

$$\bar{x} = \frac{1}{q} \sum_{i=1}^q x_i \quad \text{and} \quad \bar{y} = \frac{1}{q} \sum_{i=1}^q y_i.$$

$$\text{French: } y = 0.0683x + 8.7253$$

$$\text{English: } y = 0.0643x - 3.5972$$



# Regression: Notation in a Two-dimensional Space

- 1 The feature vector (or predictors):  $(1, x_1, x_2, \dots, x_{n-1})$  representing the input. In our example, this corresponds to the letter frequencies:  $(1, 36961)$  in Chapter 1. The first parameter is set to 1;
- 2 The output (or response or target):  $y$ . In our example, the frequencies of  $a$ : 2503 in Chapter 1; the predicted output:  
$$\hat{y} = 0.0683 \times 36961 + 8.7253 = 2533.22$$
- 3 The squared error for one point:  $(2503 - 2533.22)^2 = 30.22^2 = 913.26$
- 4 To denote the whole data set, we use a matrix,  $\mathbf{X}$ , where each row corresponds to an observation and a vector  $\mathbf{y}$  for the outputs



# Complete Matrix

For the French dataset, the complete matrix and vectors are:

$$\mathbf{X} = \begin{bmatrix} 1 & 36961 \\ 1 & 43621 \\ 1 & 15694 \\ 1 & 36231 \\ 1 & 29945 \\ 1 & 40588 \\ 1 & 75255 \\ 1 & 37709 \\ 1 & 30899 \\ 1 & 25486 \\ 1 & 37497 \\ 1 & 40398 \\ 1 & 74105 \\ 1 & 76725 \\ 1 & 18317 \end{bmatrix} ; \mathbf{w} = \begin{bmatrix} 8.7253 \\ 0.0683 \end{bmatrix} ; \hat{\mathbf{y}} = \begin{bmatrix} 2533.22 \\ 2988.11 \\ 1080.65 \\ 2483.36 \\ 2054.02 \\ 2780.95 \\ 5148.76 \\ 2584.31 \\ 2119.18 \\ 1749.46 \\ 2569.83 \\ 2767.97 \\ 5070.21 \\ 5249.16 \\ 1259.81 \end{bmatrix} ; \mathbf{y} = \begin{bmatrix} 2503 \\ 2992 \\ 1042 \\ 2487 \\ 2014 \\ 2805 \\ 5062 \\ 2643 \\ 2126 \\ 1784 \\ 2641 \\ 2766 \\ 5047 \\ 5312 \\ 1215 \end{bmatrix} ; \mathbf{se} = \begin{bmatrix} 913.26 \\ 15.14 \\ 1493.86 \\ 13.25 \\ 1601.31 \\ 578.40 \\ 7527.51 \\ 3444.53 \\ 46.57 \\ 1193.04 \\ 5065.18 \\ 38920 \\ 538.909 \\ 3948.29 \\ 2007.53 \end{bmatrix} .$$

# Regression: Notation in an $N$ -dimensional Space

The least-squares method minimizes the sum of the squared errors for all the observations through optimal values of  $m$  and  $b$ . In an  $n$ -dimensional space, we have:

- ❶ The weight vector:  $(w_0, w_1, w_2, \dots, w_{n-1})$ ,  $(8.7253, 0.0683)$  for French and  $(-3.5972, 0.0643)$  for English;
- ❷ The intercept:  $w_0$ .

The hyperplane equation corresponds to the dot product of the weights by the features defined as:

$$y = \mathbf{w} \cdot \mathbf{x} = \sum_{i=0}^{n-1} w_i x_i,$$

where  $\mathbf{w} = (w_0, w_1, w_2, \dots, w_{n-1})$ ,  $\mathbf{x} = (x_0, x_1, x_2, \dots, x_{n-1})$ , and  $x_0 = 1$ .



# Another Technique: The Gradient Descent

The gradient descent is a numerical method to find the minimum of  $f(x_0, x_1, x_2, \dots, x_n) = y$ , when there is no analytical solution.

Let us denote  $\mathbf{x} = (x_0, x_1, x_2, \dots, x_n)$

We derive successive approximations to find the minimum of  $f$ :

$$f(\mathbf{x}_1) > f(\mathbf{x}_2) > \dots > f(\mathbf{x}_k) > f(\mathbf{x}_{k+1}) > \dots > \min$$

Points in the neighborhood of  $\mathbf{x}$  are defined by  $\mathbf{x} + \mathbf{v}$  with  $\|\mathbf{v}\|$  small

Given  $\mathbf{x}$ , find  $\mathbf{v}$  subject to  $f(\mathbf{x}) > f(\mathbf{x} + \mathbf{v})$



# The Gradient Descent (Cauchy, 1847)

Using a Taylor expansion:  $f(\mathbf{x} + \mathbf{v}) = f(\mathbf{x}) + \mathbf{v} \cdot \nabla f(\mathbf{x}) + \dots$

The gradient is a direction vector corresponding to the steepest slope:

$$\nabla f(x_0, x_1, x_2, \dots, x_n) = \left( \frac{\partial f}{\partial x_0}, \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right).$$

$f(\mathbf{x} + \mathbf{v})$  reaches a minimum or a maximum when  $\mathbf{v}$  and  $\nabla f(\mathbf{x})$  are colinear:

- Steepest ascent:  $\mathbf{v} = \alpha \nabla f(\mathbf{x})$ ,
- Steepest descent:  $\mathbf{v} = -\alpha \nabla f(\mathbf{x})$ ,

where  $\alpha > 0$ .

We have then:  $f(\mathbf{x} - \alpha \nabla f(\mathbf{x})) \approx f(\mathbf{x}) - \alpha \|\nabla f(\mathbf{x})\|^2$ .

The inequality:

$$f(\mathbf{x}) > f(\mathbf{x} - \alpha \nabla f(\mathbf{x}))$$

enables us to move one step down to the minimum.

We then use the iteration:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \nabla f(\mathbf{x}_k).$$



# Algorithm

For a data set  $DS$ , we find the minimum through a walk (iteration) down the surface.

```

1: function Regression( $DS$ )
2:    $\mathbf{w} \leftarrow \mathbf{w}^0$ 
3:   while  $\|\nabla \text{Loss}(\mathbf{w})\| > \varepsilon$  do
4:      $\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla \text{Loss}(\mathbf{w})$ 
5:   return  $\mathbf{w}$ 

```

▷  $\mathbf{w}^0$ : Any point in the space

$\alpha$  is a positive number either constant or variable.



# In a Two-dimensional Space

To make the generalization easier, let us rename the straight line coefficients  $(b, m)$  as  $(w_0, w_1)$

Given a data set  $DS$  of  $q$  examples:  $DS = \{(1, x_1^j, y^j) | j : 1..q\}$ , where the error is defined as:

$$\begin{aligned} SSE(w_0, w_1) &= \sum_{j=1}^q (y^j - \hat{y}^j)^2 \\ &= \sum_{j=1}^q (y^j - (w_0 + w_1 x_1^j))^2. \end{aligned}$$

The gradient with  $q$  examples:

$$\begin{aligned} \frac{\partial SSE}{\partial w_0} &= -2 \sum_{j=1}^q (y^j - (w_0 + w_1 x_1^j)) \\ \frac{\partial SSE}{\partial w_1} &= -2 \sum_{j=1}^q x_1^j \times (y^j - (w_0 + w_1 x_1^j)) \end{aligned}$$





# Updates

Batch gradient descent with  $q$  examples:

$$w_0 \leftarrow w_0 + \frac{\alpha}{q} \sum_{j=1}^q (y^j - (w_0 + w_1 x_1^j))$$

$$w_1 \leftarrow w_1 + \frac{\alpha}{q} \sum_{j=1}^q x_1^j \times (y^j - (w_0 + w_1 x_1^j))$$

Stochastic gradient descent. The updates are carried out one example at a time:

$$w_0 \leftarrow w_0 + \alpha \cdot (y^j - (w_0 + w_1 x_1^j))$$

$$w_1 \leftarrow w_1 + \alpha \cdot x_1^j \cdot (y^j - (w_0 + w_1 x_1^j))$$

The stochastic variant is also called online learning and is usually faster.



# The Gradient Descent and Linear Regression

In the general case, we want to find the regression hyperplane:

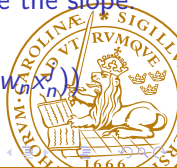
$$\hat{y} = w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n$$

given a data set of  $q$  examples:  $DS = \{(1, x_1^j, x_2^j, \dots, x_n^j, y^j) | j : 1..q\}$ , where the loss is defined as:

$$\begin{aligned} Loss(w_0, w_1, \dots, w_n) &= \sum_{j=1}^q (y^j - \hat{y}^j)^2 \\ &= \sum_{j=1}^q (y^j - (w_0 + w_1x_1^j + w_2x_2^j + \dots + w_nx_n^j))^2 \end{aligned}$$

We introduce  $x_0 = 1$  and we compute the gradient to determine the slope:

$$\frac{\partial Loss}{\partial w_i} = -2 \sum_{j=1}^q x_i^j \times (y^j - (w_0x_0^j + w_1x_1^j + w_2x_2^j + \dots + w_nx_n^j))$$



# Updates

In the **batch gradient descent**, the iteration step considers all the examples,  $q$  examples here:

$$w_i \leftarrow w_i + \frac{\alpha}{q} \cdot \sum_{j=1}^q x_i^j \cdot (y^j - (w_0 x_0^j + w_1 x_1^j + w_2 x_2^j + \dots + w_n x_n^j))$$

Using a matrix notation:

$$\mathbf{w} \leftarrow \mathbf{w} + \frac{\alpha}{q} \mathbf{X}^T \cdot (\mathbf{y} - \mathbf{X}\mathbf{w}).$$

In the **stochastic gradient descent**, we carry out the updates using one example at a time:

$$w_i \leftarrow w_i + \alpha \cdot x_i^j \cdot (y^j - (w_0 x_0^j + w_1 x_1^j + w_2 x_2^j + \dots + w_n x_n^j))$$

Using a vector notation with  $\mathbf{x}^j$  and  $y^j$ , we have:

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha \cdot (y^j - \mathbf{x}^j \cdot \mathbf{w}) \cdot \mathbf{x}^j.$$



# Definitions

An epoch is the period corresponding to one iteration over the complete data set: the  $q$  examples.

$\alpha$  is called the learning rate or the step size. It is a positive number that is either fixed or varies (decreases) over the epochs.

Setting  $\alpha$  can be difficult. In the assignments, you will manually try a set of values and check the convergence.

Murphy (2012) describes other methods (for logistic regression). See Sect. 8.3.2 and 8.5.2. They are outside the scope of this course.

See also the articles published by the LIBLINEAR team:

<http://www.csie.ntu.edu.tw/~cjlin/liblinear/>.



# The Analytical Solution Again

In a two-dimensional space, linear regression has an analytical solution:

$$m = \frac{\sum_{i=1}^q x_i y_i - q \bar{x} \bar{y}}{\sum_{i=1}^q x_i^2 - q \bar{x}^2} \quad \text{and} \quad b = \bar{y} - m \bar{x}.$$

This can be generalized for any dimension.

Let  $\mathbf{X} = (\mathbf{x}^1; \mathbf{x}^2; \dots; \mathbf{x}^q)$  be our observations and  $\mathbf{y}$ , the output. We have:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}}$$

We minimize the sum of squared errors with:

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

$(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$  is called the pseudo-inverse.



# Inverting $\mathbf{X}^T\mathbf{X}$

But:  $\mathbf{X}^T\mathbf{X}$  may be singular.

We have the property:  $\mathbf{X}^T\mathbf{X}$  is invertible if  $\mathbf{X}$  has linearly independent columns.

This means that: Singular matrices occur with highly correlated features (or duplicate ones).

A way to solve it is to add it a scalar matrix (Hoerl, 1962):

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

Equivalent to adding the term  $\lambda \|\mathbf{w}\|^2$  to the sum of squared errors (SSE).

This process is called a regularization. It is also used in classification



# Regularization

Correlated features result in large values of  $\mathbf{w}$  that regularization tries to penalize.

We replace *Loss* with a *Cost*:

$$\text{Cost}(\mathbf{w}) = \text{Loss}(\mathbf{w}) + \lambda L_q(\mathbf{w}),$$

where

$$L_q = \sum_{i=1}^n |w_i|^q.$$

The most frequent regularizations are (ridge regression):

$$L_2 = \sum_{i=1}^n w_i^2,$$

and (LASSO regression)

$$L_1 = \sum_{i=1}^n |w_i|.$$

$w_0$  may be part of the regularization.



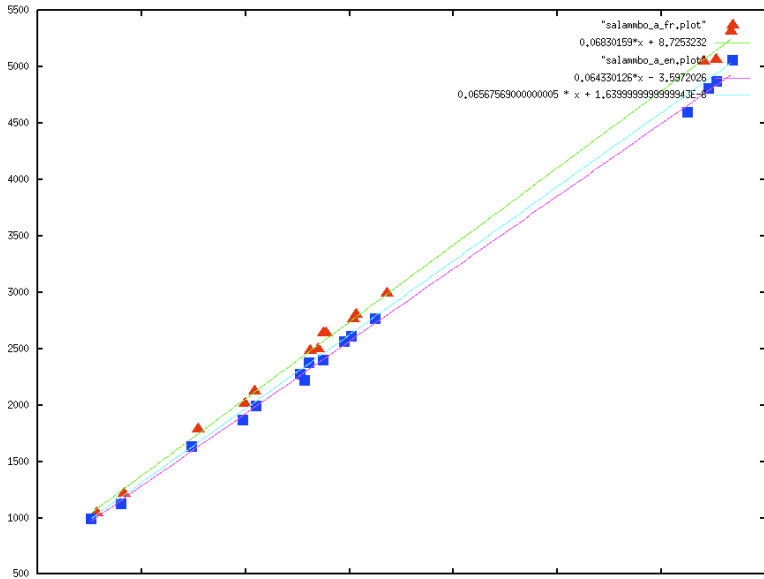
# Classification vs. Regression

- Regression:** Given an input, compute a continuous numerical output.  
For instance compute the number of *A* occurring in a text in French from the total number of characters.  
Having 75,255 characters in Chapter 7, the regression line will predict 5,149 occurrences of *A* (5,062 in reality).
- Classification:** Given the number of characters and the number of *A* in a text, predict the language: French or English.  
For instance, having the pair (75255, 5062), the classifier will predict French.  
The classification output is a finite set of values. When there are two values, we have a binary classification.





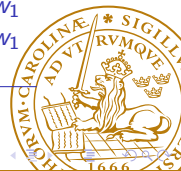
# Separating Classes



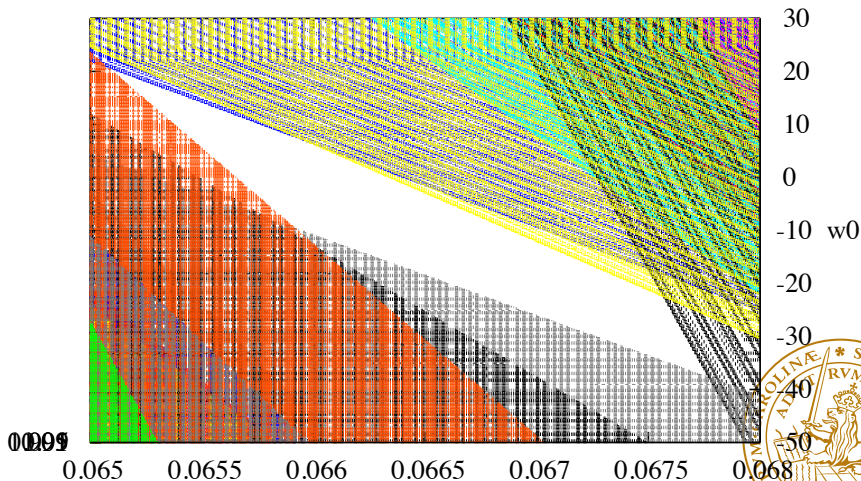
# Classification: An Example

$y_i > w_0 + w_1 x_i$  for the set of points:  $\{(x_i, y_i) | (x_i, y_i) \in \text{French}\}$  and  
 $y_i < w_0 + w_1 x_i$  for the set of points:  $\{(x_i, y_i) | (x_i, y_i) \in \text{English}\},$

| Chapter | French                   | English                  |
|---------|--------------------------|--------------------------|
| 1       | $2503 > w_0 + 36961 w_1$ | $2217 < w_0 + 35680 w_1$ |
| 2       | $2992 > w_0 + 43621 w_1$ | $2761 < w_0 + 42514 w_1$ |
| 3       | $1042 > w_0 + 15694 w_1$ | $990 < w_0 + 15162 w_1$  |
| 4       | $2487 > w_0 + 36231 w_1$ | $2274 < w_0 + 35298 w_1$ |
| 5       | $2014 > w_0 + 29945 w_1$ | $1865 < w_0 + 29800 w_1$ |
| 6       | $2805 > w_0 + 40588 w_1$ | $2606 < w_0 + 40255 w_1$ |
| 7       | $5062 > w_0 + 75255 w_1$ | $4805 < w_0 + 74532 w_1$ |
| ...     |                          |                          |

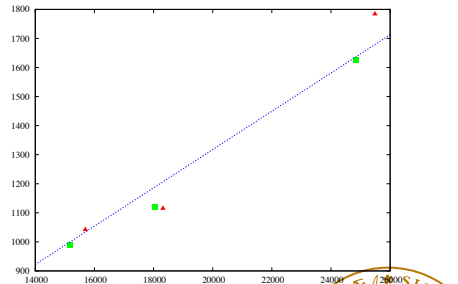
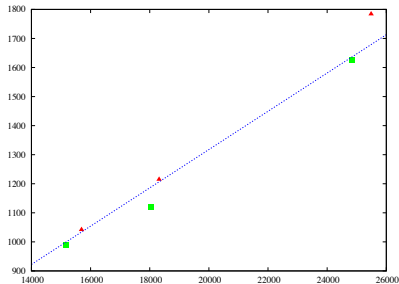


# The Inequality System



# Separability

Linear classification is based on the linear separability of the classes.  
This is not always the case



# Dimension of the Feature Space

Regression predicts the value of one of the features given the value of  $N - 1$  features.

Classification predicts the class given the values of  $N$  features.

Compared to regression in our example, the dimension of the vector space used for the classification is  $N + 1$ : The  $N$  features and the class.

| # characters | # A   | Language |
|--------------|-------|----------|
| 36,961       | 2,503 | French   |
| 35,680       | 2,217 | English  |
| 43,621       | 2,992 | French   |
| 42,514       | 2,761 | English  |
| 15,694       | 1,042 | French   |
| 15,162       | 990   | English  |
| 36,231       | 2,487 | French   |
| 35,298       | 2,274 | English  |
| etc.         |       |          |



# Classification

We represent classification using a threshold function (a variant of the signum function):

$$H(\mathbf{w} \cdot \mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{x} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The classification function associates  $P$  with 1 and  $N$  with 0.  
We want to find the separating hyperplane:

$$\begin{aligned} \hat{y}(\mathbf{x}) &= H(\mathbf{w} \cdot \mathbf{x}) \\ &= H(w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n), \end{aligned}$$

given a data set of  $q$  examples:  $DS = \{(1, x_1^j, x_2^j, \dots, x_n^j, y^j) | j : 1..q\}$ .

We use  $x_0 = 1$  to simplify the equations.

For a binary classifier,  $y$  has then two possible values  $\{0, 1\}$  corresponding in our example to  $\{\text{French, English}\}$ .



# Loss Function

To assess the classification, we use the 0/1 loss defined as

$$L_{0/1}(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ 1 & \text{otherwise} \end{cases}$$

The update rule of linear regression is:

$$w_i \leftarrow w_i + \alpha \cdot \sum_{j=1}^q x_i^j \cdot (y^j - \hat{y}^j)$$

$$w_i \leftarrow w_i + \alpha \cdot \sum_{j=1}^q x_i^j \cdot (y^j - (w_0 x_0^j + w_1 x_1^j + w_2 x_2^j + \dots + w_n x_n^j))$$

Using the same idea, we compute the weight updates of a classification as:

$$w_i \leftarrow w_i + \alpha \sum_{j=1}^q x_i^j \cdot (y^j - \hat{y}^j)$$



# The Perceptron Learning Rule

If all the points are correctly classified, there is no update:  $y^j - \hat{y}^j = 0$ , either  $0 - 0$  or  $1 - 1$

The loss involves an update only for the misclassified points, either  $1 - 0$  or  $0 - 1$

The update is then:  $\alpha \cdot x_i$  or  $-\alpha \cdot x_i$

$\alpha$  is generally set to 1 as a division of the weight vector by a constant does not affect the update rule

The perceptron is usually trained one example at a time: stochastic learning  
Examples should be selected randomly





# In a Two-dimensional Space

Classification with two classes:

$$w_0 + w_1x_1 + w_2x_2 > 0$$

$$w_0 + w_1x_1 + w_2x_2 < 0,$$

Vectors:

$$\mathbf{x} = (1, x_1, x_2) \quad \text{and} \quad \mathbf{w} = (w_0, w_1, w_2)$$

Stochastic gradient descent. The updates are carried out one example at a time:

$$w_0 \leftarrow w_0 + (y^j - \hat{y}^j)$$

$$w_1 \leftarrow w_1 + x_1^j \cdot (y^j - \hat{y}^j)$$

$$w_2 \leftarrow w_2 + x_2^j \cdot (y^j - \hat{y}^j)$$

where  $y^j - \hat{y}^j$  is either, 0, -1, or 1.



# Stop Conditions

To find a hyperplane, the examples must be separable. This is rarely the case in practice

Workaround:

- Stop learning when the number of misclassified examples is low
- Use  $\alpha(t) = \frac{1000}{1000 + t}$  instead of a fixed value. (According to the book)



# Matrix Notation

- A feature vector (predictors):  $\mathbf{x}$ , and feature matrix:  $\mathbf{X}$ ;
- The class:  $y$  and the class vector:  $\mathbf{y}$ ;
- The predicted class (response):  $\hat{y}$ , and predicted class vector:  $\hat{\mathbf{y}}$

$$\mathbf{X} = \begin{bmatrix} \text{Sunny} & \text{Hot} & \text{High} & \text{False} \\ \text{Sunny} & \text{Hot} & \text{High} & \text{True} \\ \text{Overcast} & \text{Hot} & \text{High} & \text{False} \\ \text{Rain} & \text{Mild} & \text{High} & \text{False} \\ \text{Rain} & \text{Cool} & \text{Normal} & \text{False} \\ \text{Rain} & \text{Cool} & \text{Normal} & \text{True} \\ \text{Overcast} & \text{Cool} & \text{Normal} & \text{True} \\ \text{Sunny} & \text{Mild} & \text{High} & \text{False} \\ \text{Sunny} & \text{Cool} & \text{Normal} & \text{False} \\ \text{Rain} & \text{Mild} & \text{Normal} & \text{False} \\ \text{Sunny} & \text{Mild} & \text{Normal} & \text{True} \\ \text{Overcast} & \text{Mild} & \text{High} & \text{True} \\ \text{Overcast} & \text{Hot} & \text{Normal} & \text{False} \\ \text{Rain} & \text{Mild} & \text{High} & \text{True} \end{bmatrix}; \mathbf{y} = \begin{bmatrix} \text{N} \\ \text{N} \\ \text{P} \\ \text{P} \\ \text{P} \\ \text{P} \\ \text{N} \\ \text{P} \\ \text{N} \\ \text{P} \\ \text{P} \\ \text{P} \\ \text{P} \\ \text{N} \end{bmatrix}$$



# Converting Symbolic Attributes into Numerical Vectors

Symbolic – nominal – attributes are mapped onto vectors of binary values.  
A conversion of the weather data set.

| Object | Attributes |          |      |             |      |      |          |        |       |       | Class |
|--------|------------|----------|------|-------------|------|------|----------|--------|-------|-------|-------|
|        | Outlook    |          |      | Temperature |      |      | Humidity |        | Windy |       |       |
|        | Sunny      | Overcast | Rain | Hot         | Mild | Cool | High     | Normal | True  | False |       |
| 1      | 1          | 0        | 0    | 1           | 0    | 0    | 1        | 0      | 0     | 1     | N     |
| 2      | 1          | 0        | 0    | 1           | 0    | 0    | 1        | 0      | 1     | 0     | N     |
| 3      | 0          | 1        | 0    | 1           | 0    | 0    | 1        | 0      | 0     | 1     | P     |
| 4      | 0          | 0        | 1    | 0           | 1    | 0    | 1        | 0      | 0     | 1     | P     |
| 5      | 0          | 0        | 1    | 0           | 0    | 1    | 0        | 1      | 0     | 1     | P     |
| 6      | 0          | 0        | 1    | 0           | 0    | 1    | 0        | 1      | 1     | 0     | N     |
| 7      | 0          | 1        | 0    | 0           | 0    | 1    | 0        | 1      | 1     | 0     | P     |
| 8      | 1          | 0        | 0    | 0           | 1    | 0    | 1        | 0      | 0     | 1     | N     |
| 9      | 1          | 0        | 0    | 0           | 0    | 1    | 0        | 1      | 0     | 1     | P     |
| 10     | 0          | 0        | 1    | 0           | 1    | 0    | 0        | 1      | 0     | 1     | P     |
| 11     | 1          | 0        | 0    | 0           | 1    | 0    | 0        | 1      | 1     | 0     | P     |
| 12     | 0          | 1        | 0    | 0           | 1    | 0    | 1        | 0      | 1     | 0     | P     |
| 13     | 0          | 1        | 0    | 1           | 0    | 0    | 0        | 1      | 0     | 1     | P     |
| 14     | 0          | 0        | 1    | 0           | 1    | 0    | 1        | 0      | 1     | 0     | N     |

This kind of transformation is called contrast coding or one-hot encoding (OHE).



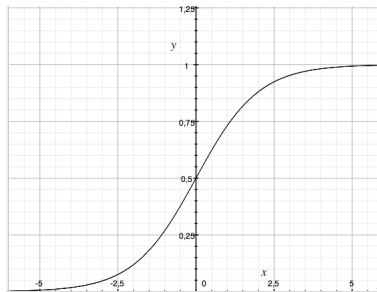
# Matrix Notation

$$\mathbf{x} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}; \mathbf{y} = \begin{bmatrix} N \\ N \\ P \\ P \\ P \\ P \\ N \\ P \\ N \\ P \\ P \\ P \\ P \\ N \end{bmatrix}$$



# Logistic Regression

The step function is not differentiable; that is why it is often replaced with the logistic curve (Verhulst, 1845, 1848):



$$\begin{aligned}\hat{y}(x) &= \text{Logistic}(w \cdot x) \\ &= \frac{1}{1 + e^{-w \cdot x}}\end{aligned}$$



# Logistic Regression: The Idea

| Drug concentration | Number exposed | Survive Class 0 | Die Class 1 | Mortality rate | Expected mortality |
|--------------------|----------------|-----------------|-------------|----------------|--------------------|
| 40                 | 462            | 352             | 110         | .2359          | .2206              |
| 60                 | 500            | 301             | 199         | .3980          | .4339              |
| 80                 | 467            | 169             | 298         | .6380          | .6085              |
| 100                | 515            | 145             | 370         | .7184          | .7291              |
| 120                | 561            | 102             | 459         | .8182          | .8081              |
| 140                | 469            | 69              | 400         | .8529          | .8601              |
| 160                | 550            | 55              | 495         | .9000          | .8952              |
| 180                | 542            | 43              | 499         | .9207          | .9195              |
| 200                | 479            | 29              | 450         | .9395          | .9366              |
| 250                | 497            | 21              | 476         | .9577          | .9624              |
| 300                | 453            | 11              | 442         | .9757          | .9756              |

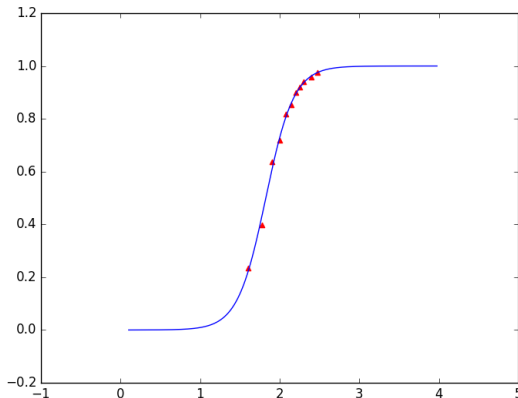
**Table:** A data set. Adapted and simplified from the original article that described how to apply logistic regression to classification by Joseph Berkson, Application of the Logistic Function to Bio-Assay. *Journal of the American Statistical Association* (1944).



# Fitting the Logistic Curve

Berkson fitted the curve to the data using the logarithm of the dose. He obtained:

$$\frac{1}{1 + e^{-5.659746x + 10.329884}}$$





# Logistic Regression

Logistic regression attempts to model the probability of an observation  $\mathbf{x}$  to belong to a class:

$$P(y = 1|\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

and

$$P(y = 0|\mathbf{x}) = \frac{e^{-\mathbf{w} \cdot \mathbf{x}}}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

These probabilities are extremely useful in practice.

The logit assumption (Berkson, 1944) models the odd ratio as a hyperplane:

$$\ln \frac{P(y = 1|\mathbf{x})}{P(y = 0|\mathbf{x})} = \ln \frac{P(y = 1|\mathbf{x})}{1 - P(y = 1|\mathbf{x})} = \mathbf{w} \cdot \mathbf{x}$$



# Likelihood of a Classification

Given a data set,  $DS$ , containing a partition in two classes,  $P$  ( $y = 1$ ) and  $N$  ( $y = 0$ ), and a model  $w$ , the likelihood to have the classification observed in this data set is:

$$\begin{aligned} L(w) &= \prod_{\mathbf{x}^j \in P} P(y^j = 1 | \mathbf{x}^j) \times \prod_{\mathbf{x}^j \in N} P(y^j = 0 | \mathbf{x}^j), \\ &= \prod_{\mathbf{x}^j \in P} P(y^j = 1 | \mathbf{x}^j) \times \prod_{\mathbf{x}^j \in N} (1 - P(y^j = 1 | \mathbf{x}^j)). \end{aligned}$$

We can rewrite the product using  $y^j$  as powers of the probabilities as  $y^j = 0$ , when  $\mathbf{x}^j \in P$  and  $y^j = 1$ , when  $\mathbf{x}^j \in N$ :

$$\begin{aligned} L(w) &= \prod_{\mathbf{x}^j \in P} P(y^j = 1 | \mathbf{x}^j)^{y^j} \times \prod_{\mathbf{x}^j \in N} (1 - P(y^j = 1 | \mathbf{x}^j))^{1-y^j}, \\ &= \prod_{(\mathbf{x}^j, y^j) \in DS} P(y^j = 1 | \mathbf{x}^j)^{y^j} \times (1 - P(y^j = 1 | \mathbf{x}^j))^{1-y^j} \end{aligned}$$



# Maximizing the Likelihood

We train a model by maximizing the likelihood of the observed classification:

$$\hat{w} = \arg \max_w \prod_{\mathbf{x}^j \in DS} P(y^j = 1 | \mathbf{x}^j)^{y^j} \times (1 - P(y^j = 1 | \mathbf{x}^j))^{1-y^j}$$

To maximize this term, it is more convenient to work with sums rather than with products and we take the logarithm of it (log-likelihood):

$$\hat{w} = \arg \max_w \sum_{(\mathbf{x}^j, y^j) \in DS} y^j \ln P(y^j = 1 | \mathbf{x}^j) + (1 - y^j) \ln(1 - P(y^j = 1 | \mathbf{x}^j))$$

Using the logistic curves to express the probabilities, we have:

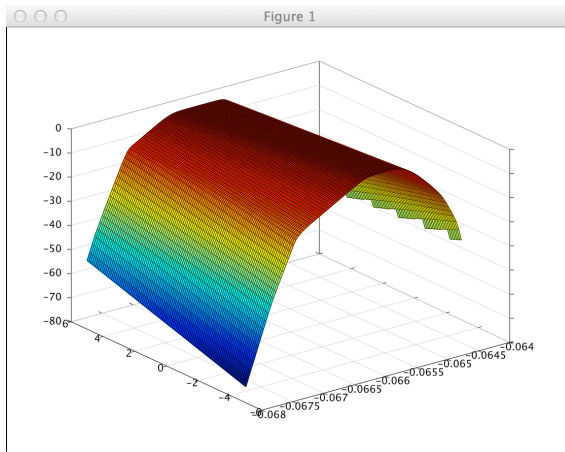
$$\hat{w} = \arg \max_w \sum_{(\mathbf{x}^j, y^j) \in DS} y^j \ln \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}} + (1 - y^j) \ln \frac{e^{-\mathbf{w} \cdot \mathbf{x}^j}}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}}.$$

In contrast to linear regression that uses least mean squares, here we fit a logistic curve so that it maximizes the likelihood of the classification partition – observed in the training set.



# The Maximum

Graph of the probabilities from the *Salammbô* data set.



The opposite is called the cross-entropy loss.



# The Gradient Ascent

We can use the gradient ascent to compute the maximum.

Using a Taylor expansion:  $\ell(\mathbf{w} + \mathbf{v}) = \ell(\mathbf{w}) + \mathbf{v} \cdot \nabla \ell(\mathbf{w}) + \dots$

We have then:  $\ell(\mathbf{w} + \alpha \nabla \ell(\mathbf{w})) \approx \ell(\mathbf{w}) + \alpha \|\nabla \ell(\mathbf{w})\|^2$ .

The inequality:

$$\ell(\mathbf{w}) < \ell(\mathbf{w} + \alpha \nabla \ell(\mathbf{w}))$$

enables us to move one step up to the maximum.

We then use the iteration:

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \alpha_k \nabla \ell(\mathbf{w}_k).$$



# Computing the Model

The partial derivatives of the log-likelihood are:

$$\begin{aligned}
 \frac{\partial \ell(\mathbf{w})}{\partial w_i} &= \sum_{(\mathbf{x}^j, y^j) \in DS} y^j (1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}) \frac{x_i^j e^{-\mathbf{w} \cdot \mathbf{x}^j}}{(1 + e^{-\mathbf{w} \cdot \mathbf{x}^j})^2} + \\
 &\quad (1 - y^j) \frac{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}}{e^{-\mathbf{w} \cdot \mathbf{x}^j}} \cdot \frac{-x_i^j \cdot e^{-\mathbf{w} \cdot \mathbf{x}^j} (1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}) + x_i^j \cdot e^{-\mathbf{w} \cdot \mathbf{x}^j} \cdot e^{-\mathbf{w} \cdot \mathbf{x}^j}}{(1 + e^{-\mathbf{w} \cdot \mathbf{x}^j})^2}, \\
 &= \sum_{(\mathbf{x}^j, y^j) \in DS} y^j \frac{x_i^j e^{-\mathbf{w} \cdot \mathbf{x}^j}}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}} + (1 - y^j) \cdot \frac{-x_i^j \cdot (1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}) + x_i^j \cdot e^{-\mathbf{w} \cdot \mathbf{x}^j}}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}}, \\
 &= \sum_{(\mathbf{x}^j, y^j) \in DS} x_i^j \cdot \frac{y^j \cdot (1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}) - 1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}}, \\
 &= \sum_{(\mathbf{x}^j, y^j) \in DS} x_i^j \cdot \left( y^j - \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}} \right).
 \end{aligned}$$



# Weight Updates

For  $DS = \{(1, x_1^j, x_2^j, \dots, x_n^j, y^j) | j : 1..q\}$ , the weight updates of logistic regression are then:

- Stochastic gradient ascent:

$$w_i \leftarrow w_i + \alpha \cdot x_i^j \cdot \left( y^j - \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}} \right)$$

- Batch gradient ascent:

$$w_i \leftarrow w_i + \frac{\alpha}{q} \cdot \sum_{j=1}^q x_i^j \cdot \left( y^j - \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}^j}} \right)$$

As with gradient descent, we stop the iterations when:

$$\|\nabla \ell(\mathbf{w})\| < \varepsilon.$$



# Loss: Binary Crossentropy

Alternatively, we can compute a loss and minimize it.

We just take the negated value of the likelihood.

We then call the corresponding function the **log-loss** or **cross entropy**

Most machine learning practitioners and toolkits use the natural logarithm and minimize the mean:

$$-\frac{1}{q} \sum_{j=1}^q (y^j \ln \hat{y}^j + (1 - y^j) \ln(1 - \hat{y}^j)).$$

Both approaches, maximum likelihood and binary crossentropy, are equivalent.

I feel the maximum likelihood one more intuitive.





# Multinomial (Multiclass) Logistic Regression

Generalizing logistic regression from

$$\ln \frac{P(y = 1|x)}{P(y = 0|x)} = \mathbf{w} \cdot \mathbf{x}$$

to a multiclass setting is easy.

Using  $y = 0$  as a pivot, we have for  $C$  classes:

$$\ln \frac{P(y = 1|x)}{P(y = 0|x)} = \mathbf{w}_1 \cdot \mathbf{x}$$

$$\ln \frac{P(y = 2|x)}{P(y = 0|x)} = \mathbf{w}_2 \cdot \mathbf{x}$$

...

$$\ln \frac{P(y = C-1|x)}{P(y = 0|x)} = \mathbf{w}_{C-1} \cdot \mathbf{x}$$

and

$$\sum_{k=0}^{C-1} P(y = k|x) = 1.$$



# Multinomial (Multiclass) Logistic Regression (II)

We obtain:

$$P(y = 0|\mathbf{x}) = \frac{1}{1 + \sum_{i=1}^{C-1} e^{\mathbf{w}_i \cdot \mathbf{x}}}$$

$$P(y = k|\mathbf{x}) = \frac{e^{\mathbf{w}_k \cdot \mathbf{x}}}{1 + \sum_{i=1}^{C-1} e^{\mathbf{w}_i \cdot \mathbf{x}}}, k = 1, 2, \dots, C-1.$$

Equivalent to:

$$P(y = k|\mathbf{x}) = \frac{e^{\mathbf{w}_k \cdot \mathbf{x}}}{\sum_{i=0}^{C-1} e^{\mathbf{w}_i \cdot \mathbf{x}}}, k = 0, 1, 2, \dots, C-1.$$

This function is often called the *softmax* function.



# Loss: Categorical Crossentropy

Binary logistic regression minimizes the crossentropy loss. Categorical crossentropy covers multiple classes. It is defined as:

$$-\frac{1}{q} \sum_{j=1}^q y_j \cdot \ln \hat{y}_j$$

where  $y_j$  corresponds to the true class of the  $j$ th observation, represented as a one-hot vector,  $\hat{y}_j$  is the probability distribution of the predicted classes. The predicted probability for  $\mathbf{x}$  to belong to class  $i$  is given by the softmax function:

$$P(y = i | \mathbf{x}) = \frac{e^{-\mathbf{w}_i \cdot \mathbf{x}}}{\sum_{j=1}^C e^{-\mathbf{w}_j \cdot \mathbf{x}}}.$$



# Neural Networks

Learning devices loosely inspired by brain neuron

Artificial neural networks abundantly use physiological metaphors, such as synapses, cortex, etc.

In our context, can be reframed as a multistage logistic regression to handle nonlinearities

Training is complex and demanding

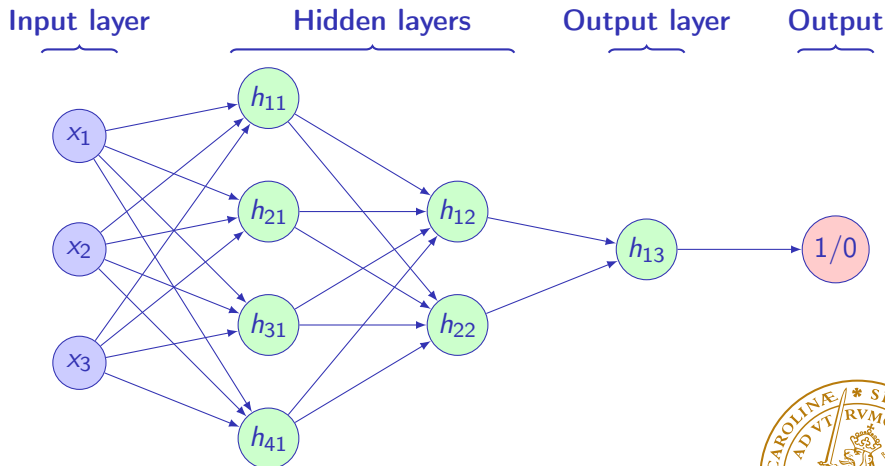
Fell out of favor in the 1990-2000s and experienced a revival with deep learning

Available programming environments include, Keras (on TensorFlow), TensorFlow, PyTorch, and PaddlePaddle:

- <https://keras.io/>
- <https://www.tensorflow.org/>
- <http://pytorch.org/>
- <http://www.paddlepaddle.org/>

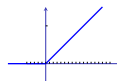


# Feed-Forward Neural Networks

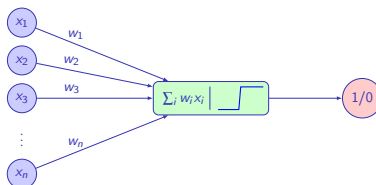


# Activation Functions

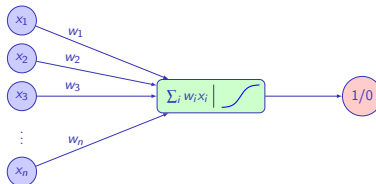
## Rectified linear unit (ReLU)



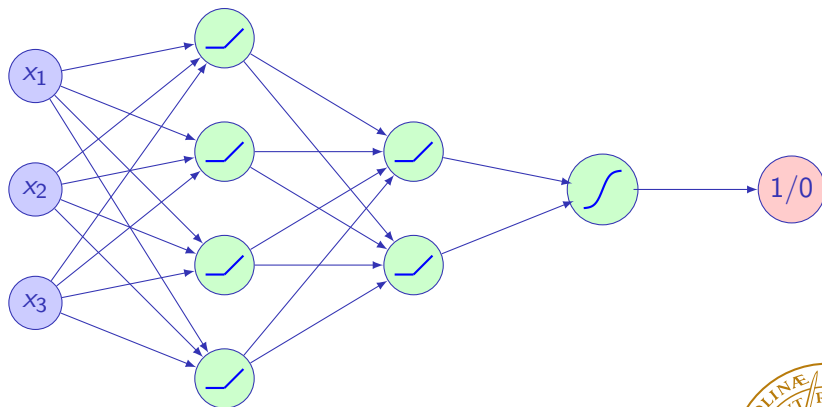
## The Perceptron



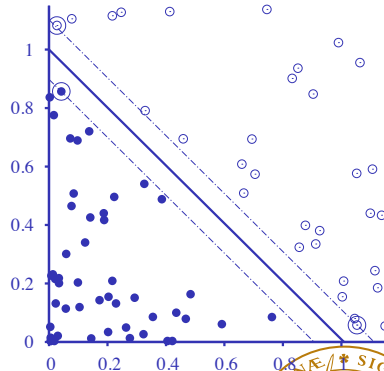
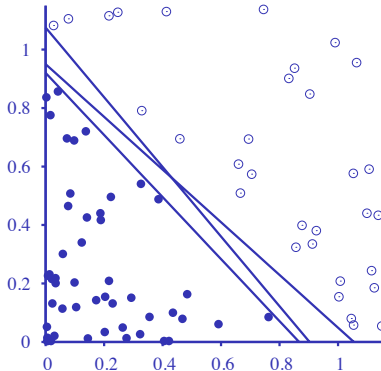
## Logistic regression



# Neural Networks with Hidden Layers



# Support Vector Machines



From the textbook: Stuart Russell and Peter Norvig, *Artificial Intelligence*, 3rd ed., 2010, page 745.





# Support Vector Machines (II)

Support vector machines (SVM) maximize the margin between the separating hyperplane and the examples

The hyperplane is set at equal distance between the closest points of each class

The closest points are called the support vectors

Support vector machines can handle nonseparable examples using a soft margin or kernels.



# Problem Description

With two classes, support vector machines use the notation:  $y = +1$  or  $y = -1$ .

We know from geometry and vector analysis that the distance of a point  $A$  to a hyperplane  $Hyp$  defined by the equation:

$$w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n = 0$$

is given by the formula:

$$d(A, Hyp) = \frac{|w_0 + w_1x_1 + w_2x_2 + \dots + w_nx_n|}{\sqrt{w_1^2 + w_2^2 + \dots + w_n^2}}.$$

We want to find the hyperplane maximizing  $b$  so that:

$$y^j \cdot \frac{w_0 + \mathbf{w} \cdot \mathbf{x}^j}{\|\mathbf{w}\|} \geq b$$

for all the points in the data set and with  $\mathbf{w} = (w_1, \dots, w_n)$ .



# Maximizing the Margin

We normalize the equation with  $b = \frac{1}{\|\mathbf{w}\|}$ .

To find the maximal margin  $b$ , we minimize  $\|\mathbf{w}\|^2$  with the constraint:

$$y^j \cdot (w_0 + \mathbf{w} \cdot \mathbf{x}^j) \geq 1,$$

where  $y^j$  values are either +1 or -1 depending on the class of the example.

We can solve this using gradient descent and hinge loss defined as:

$$\max\{0, 1 - y\mathbf{w}^T \mathbf{x}\}, \quad y \in \{-1, +1\},$$

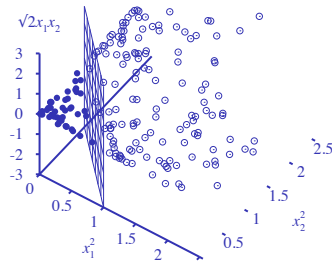
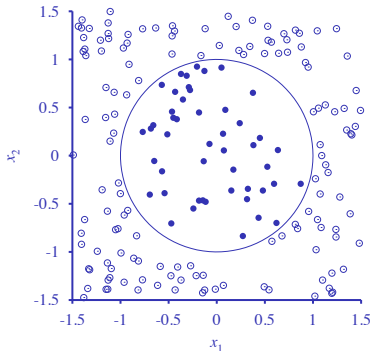
where the gradient is defined as:

$$\nabla L_{\text{hinge}} = \begin{cases} -y \cdot \mathbf{x} & \text{if } y\mathbf{w}^T \mathbf{x} < 1, \\ 0 & \text{otherwise.} \end{cases}$$



# Kernels

Many data sets are not linearly separable as in left-hand side figure.



From the textbook: Stuart Russell and Peter Norvig, *Artificial Intelligence*, 3rd ed., 2010, page 747.

It is always possible to find a space of higher dimension, where the points will be separable, here 3.



# The Kernel Trick

If we map the input data  $(x_1, x_2)$  to  $(x_1^2, x_2^2, \sqrt{2}x_1x_2)$ , we produce linearly separable classes:

$$F(x_1, x_2) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

We replace  $\mathbf{x}_j \cdot \mathbf{x}_t$  with  $F(\mathbf{x}_j) \cdot F(\mathbf{x}_t)$  in the Lagrangian:

$$L(\alpha) = \sum_{j=1}^q \alpha_j - \frac{1}{2} \sum_{j,t} \alpha_j \alpha_t y^j y^t F(\mathbf{x}_j) \cdot F(\mathbf{x}_t).$$

In the case of  $F$ , we have

$$\begin{aligned} F(\mathbf{x}) \cdot F(\mathbf{z}) &= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2 \\ &= (\mathbf{x} \cdot \mathbf{z})^2 \end{aligned}$$

In many cases, we can replace  $\mathbf{x}_j \cdot \mathbf{x}_t$  with a kernel function  $K(\mathbf{x}_j, \mathbf{x}_t)$  like  $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x} \cdot \mathbf{z})^2$



# Ensemble Learning

Idea: Use many classifiers instead of one

Boosting is an example of ensemble learning

Uses a set of  $K$  weak classifiers and gives a weight to the examples:  $w(i)$

This means that example  $i$  counts as  $w(i)$  examples

Decision stumps (decision trees with one level) are popular weak classifiers

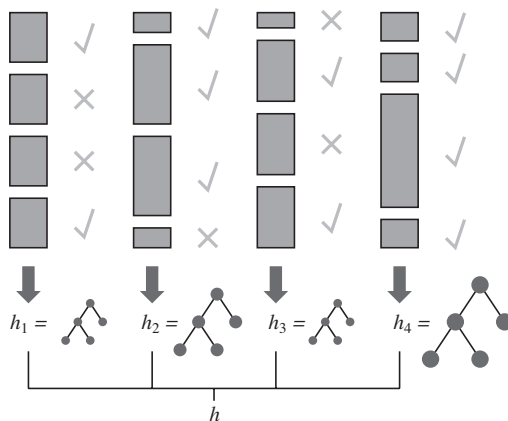
The idea of the AdaBoost algorithm is:

- 1 Learn a first stump on the training set. Each example has a weight of 1
- 2 Set a higher weight to misclassified examples (think of just duplicating them in the data set)
- 3 Learn a second decision stump.
- 4 and so on until we have  $K$  decision stumps

The final classifier is a weighted combination of the  $K$  classifiers where the weights are computed from the performance of each individual classifier



# Ensemble Learning



From the textbook: Stuart Russell and Peter Norvig, *Artificial Intelligence*, 3rd ed., 2010, page 750.

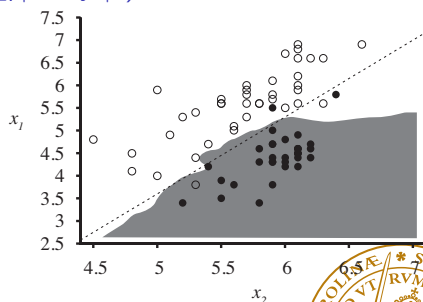
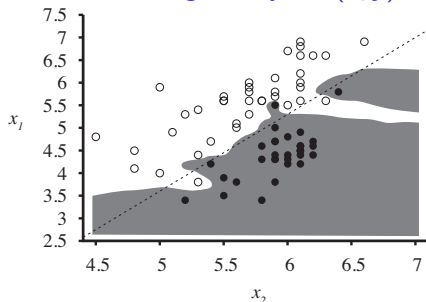


# Nonparametric Models

When there is no parametric model, such as a hyperplane, we can try to search the  $k$  nearest neighbors of  $\mathbf{x}$ :  $NN(k, \mathbf{x})$

Given a position in the space, we decide on a class by looking at the neighbor's class

The distance is given by:  $L^p(\mathbf{x}, \mathbf{y}) = (\sum_i |x_i - y_i|^p)^{\frac{1}{p}}$

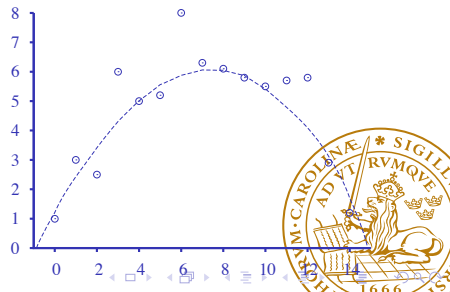
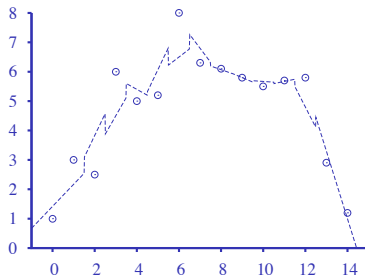
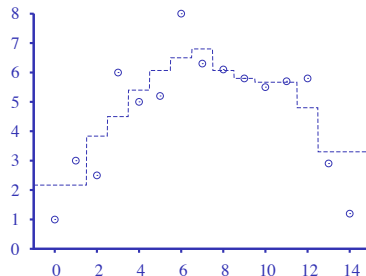
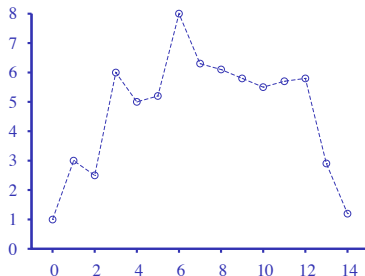


$k$  nearest neighbors with  $k = 1$  and  $k = 5$ . From the textbook: Stuart Russell and Peter Norvig, *Artificial Intelligence*, 3rd ed., 2010, page 738





# Nonparametric Regression



# scikit-learn

scikit-learn is a popular and comprehensive machine-learning library in Python built on top of numpy.

The classifiers use two main functions: `fit()` to train a model and `predict()` to predict a class. In the scikit-learn documentation, the functions adopt a notation, where:

- $x$  denotes a feature vector (the predictors) describing one observation and  $\mathbf{X}$ , a feature matrix representing the dataset;
- $y$  denotes the class (or response or target) of one observation and  $\mathbf{y}$ , the class vector for the whole dataset.



# scikit-learn: Data

```
import numpy as np

y_train = np.array(
    [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
     1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1])

X_train = np.array(
    [[35680, 2217], [42514, 2761], [15162, 990], [35298, 2274],
     [29800, 1865], [40255, 2606], [74532, 4805], [37464, 2396],
     [31030, 1993], [24843, 1627], [36172, 2375], [39552, 2560],
     [72545, 4597], [75352, 4871], [18031, 1119], [36961, 2503],
     [43621, 2992], [15694, 1042], [36231, 2487], [29945, 2014],
     [40588, 2805], [75255, 5062], [37709, 2643], [30899, 2126],
     [25486, 1784], [37497, 2641], [40398, 2766], [74105, 5047],
     [76725, 5312], [18317, 1215]
    ])
```





# scikit-learn: Crossvalidation

scikit-learn has built-in cross validation functions. The code below shows an example of it with a 5-fold cross validation and a score corresponding to the accuracy:

```
from sklearn.model_selection import cross_val_score

scores = cross_val_score(classifier, X_train, y_train, cv=5,
                          scoring='accuracy')
print('Score', scores.mean())
```



## scikit-learn: Nominal Data

|                |          |      |        |       |   |                |   |
|----------------|----------|------|--------|-------|---|----------------|---|
| $\mathbf{X} =$ | Sunny    | Hot  | High   | False | ; | $\mathbf{y} =$ | N |
|                | Sunny    | Hot  | High   | True  |   | N              |   |
|                | Overcast | Hot  | High   | False |   | P              |   |
|                | Rain     | Mild | High   | False |   | P              |   |
|                | Rain     | Cool | Normal | False |   | P              |   |
|                | Rain     | Cool | Normal | True  |   | N              |   |
|                | Overcast | Cool | Normal | True  |   | P              |   |
|                | Sunny    | Mild | High   | False |   | N              |   |
|                | Sunny    | Cool | Normal | False |   | P              |   |
|                | Rain     | Mild | Normal | False |   | P              |   |
|                | Sunny    | Mild | Normal | True  |   | P              |   |
|                | Overcast | Mild | High   | True  |   | P              |   |
|                | Overcast | Hot  | Normal | False |   | P              |   |
|                | Rain     | Mild | High   | True  |   | N              |   |



# Converting Symbolic Attributes into Numerical Vectors

Linear classifiers are numerical systems.

Symbolic – nominal – attributes are mapped onto vectors of binary values.  
A conversion of the weather data set.

| Object | Attributes |          |      |             |      |      |          |        |       |       | Class |
|--------|------------|----------|------|-------------|------|------|----------|--------|-------|-------|-------|
|        | Outlook    |          |      | Temperature |      |      | Humidity |        | Windy |       |       |
|        | Sunny      | Overcast | Rain | Hot         | Mild | Cool | High     | Normal | True  | False |       |
| 1      | 1          | 0        | 0    | 1           | 0    | 0    | 1        | 0      | 0     | 1     | N     |
| 2      | 1          | 0        | 0    | 1           | 0    | 0    | 1        | 0      | 1     | 0     | N     |
| 3      | 0          | 1        | 0    | 1           | 0    | 0    | 1        | 0      | 0     | 1     | P     |
| 4      | 0          | 0        | 1    | 0           | 1    | 0    | 1        | 0      | 0     | 1     | P     |
| 5      | 0          | 0        | 1    | 0           | 0    | 1    | 0        | 1      | 0     | 1     | P     |
| 6      | 0          | 0        | 1    | 0           | 0    | 1    | 0        | 1      | 1     | 0     | N     |
| 7      | 0          | 1        | 0    | 0           | 0    | 1    | 0        | 1      | 1     | 0     | P     |
| 8      | 1          | 0        | 0    | 0           | 1    | 0    | 1        | 0      | 0     | 1     | N     |
| 9      | 1          | 0        | 0    | 0           | 0    | 1    | 0        | 1      | 0     | 1     | P     |
| 10     | 0          | 0        | 1    | 0           | 1    | 0    | 0        | 1      | 0     | 1     | P     |
| 11     | 1          | 0        | 0    | 0           | 1    | 0    | 0        | 1      | 1     | 0     | P     |
| 12     | 0          | 1        | 0    | 0           | 1    | 0    | 1        | 0      | 1     | 0     | N     |
| 13     | 0          | 1        | 0    | 1           | 0    | 0    | 0        | 1      | 0     | 0     | N     |
| 14     | 0          | 0        | 1    | 0           | 1    | 0    | 1        | 0      | 1     | 0     | N     |



# scikit-learn: Vectorizing the Data

To convert the data to numbers, store  $\mathbf{X}$  in a list of dictionaries and use DictVectorizer:

```
from sklearn.feature_extraction import DictVectorizer  
  
vec = DictVectorizer(sparse=False) # Should be true  
X = vec.fit_transform(X_dict)
```





# scikit-learn: Data Vectorization

```
array([[ 1.,  0.,  0.,  0.,  1.,  0.,  1.,  0.,  1.,  0.],
       [ 1.,  0.,  0.,  0.,  1.,  0.,  1.,  0.,  0.,  1.],
       [ 1.,  0.,  1.,  0.,  0.,  0.,  1.,  0.,  1.,  0.],
       [ 1.,  0.,  0.,  1.,  0.,  0.,  0.,  1.,  1.,  0.],
       [ 0.,  1.,  0.,  1.,  0.,  1.,  0.,  0.,  1.,  0.],
       [ 0.,  1.,  0.,  1.,  0.,  1.,  0.,  0.,  0.,  1.],
       [ 0.,  1.,  1.,  0.,  0.,  1.,  0.,  0.,  0.,  1.],
       [ 1.,  0.,  0.,  0.,  1.,  0.,  0.,  1.,  1.,  0.],
       [ 0.,  1.,  0.,  0.,  1.,  1.,  0.,  0.,  1.,  0.],
       [ 0.,  1.,  0.,  1.,  0.,  0.,  0.,  1.,  1.,  0.],
       [ 0.,  1.,  0.,  0.,  1.,  0.,  0.,  1.,  0.,  1.],
       [ 1.,  0.,  1.,  0.,  0.,  0.,  0.,  1.,  0.,  0.],
       [ 0.,  1.,  1.,  0.,  0.,  0.,  1.,  0.,  1.,  0.],
       [ 1.,  0.,  0.,  1.,  0.,  0.,  0.,  1.,  0.,  0.]])
```



# Further Resources

**A fine videolecture:** Peter Norvig, *Statistical Learning as the Ultimate Agile Development Tool*

[http://videlectures.net/cikm08\\_norvig\\_slatuad/](http://videlectures.net/cikm08_norvig_slatuad/)

**An interesting paper:** Pedro Domingos, A Few Useful Things to Know about Machine Learning. *Communications of the ACM*, 55 (10), 78-87, 2012

**Online courses:** [openclassroom.stanford.edu](https://openclassroom.stanford.edu), [udacity.com](https://udacity.com), [coursera.org](https://coursera.org), [edx.org](https://edx.org), etc.

**Books:** Two excellent books to go further: *An Introduction to Statistical Learning with Applications in R* (start with this one) and *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*

<http://web.stanford.edu/~hastie/pub.htm>

**Tips from the expert:** An interview with #1 on Kaggle:

<http://blog.kaggle.com/2018/05/07/>

profiling-top-kagglers-bestfitting-currently-1-in-t

