

Machine Learning

2. Logistic Regression and LDA

Lars Schmidt-Thieme

Information Systems and Machine Learning Lab (ISMLL) Institute for Business Economics and Information Systems & Institute for Computer Science University of Hildesheim http://www.ismll.uni-hildesheim.de

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 1/40

Machine Learning



1. The Classification Problem

- 2. Logistic Regression
- 3. Multi-category Targets
- 4. Linear Discriminant Analysis

Classification / Supervised Learning

Example: classifying iris plants (Anderson 1935).

150 iris plants (50 of each species):

- species: setosa, versicolor, virginica
- length and width of sepals (in cm)
- length and width of petals (in cm)





iris setosa

iris versicolor



iris virginica

See iris species database (http://www.badbear.com/signa).

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 1/40

Classification / Supervised Learning

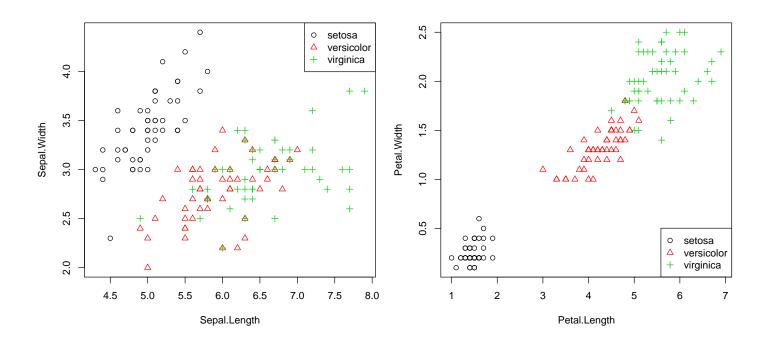
Machine Learning / 1. The Classification Problem

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.10	3.50	1.40	0.20	setosa
2	4.90	3.00	1.40	0.20	setosa
3	4.70	3.20	1.30	0.20	setosa
4	4.60	3.10	1.50	0.20	setosa
5	5.00	3.60	1.40	0.20	setosa
:	:	:	:	:	
51	7.00	3.20	4.70	1.40	versicolor
52	6.40	3.20	4.50	1.50	versicolor
53	6.90	3.10	4.90	1.50	versicolor
54	5.50	2.30	4.00	1.30	versicolor
:	:	:	:	:	
101	6.30	3.30	6.00	2.50	virginica
102	5.80	2.70	5.10	1.90	virginica
103	7.10	3.00	5.90	2.10	virginica
104	6.30	2.90	5.60	1.80	virginica
105	6.50	3.00	5.80	2.20	virginica
:	:	:	:	:	_
150	5.90	3.00	5.10	1.80	virginica

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 2/40



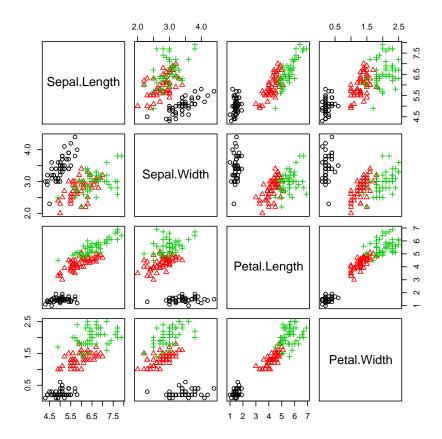
Classification / Supervised Learning



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 3/40

Machine Learning / 1. The Classification Problem

Classification / Supervised Learning



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 4/40









- 1. The Classification Problem
- 2. Logistic Regression
- 3. Multi-category Targets
- 4. Linear Discriminant Analysis

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 5/40

Machine Learning / 2. Logistic Regression

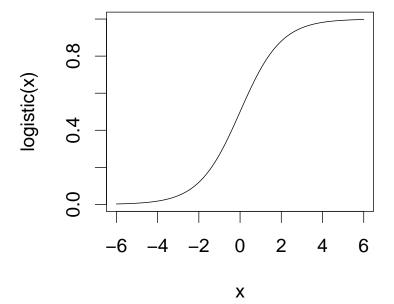
The Logistic Function

Logistic function:

$$\operatorname{logistic}(x):=\frac{e^x}{1+e^x}=\frac{1}{1+e^{-x}}$$

The logistic function is a function that

- has values between 0 and 1,
- \bullet converges to 1 when approaching $+\infty,$
- \bullet converges to 0 when approaching $-\infty,$
- is smooth and symmetric.

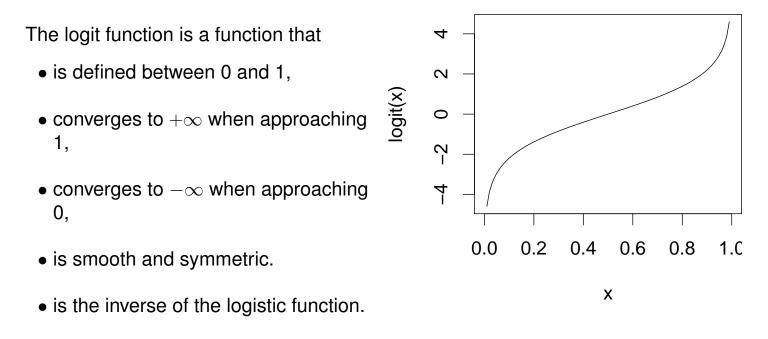


The Logit Function



Logit function:

$$\mathsf{logit}(x) := \log(\frac{x}{1-x})$$



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 6/40

Machine Learning / 2. Logistic Regression

Logistic Regression Model



Make it simple:

• target Y is binary: $\mathcal{Y} := \{0, 1\}$.

The linear regression model

$$Y = \langle X, \beta \rangle + \epsilon$$

is not suited for predicting y as it can assume all kinds of intermediate values.

Instead of predicting Y directly, we predict

p(Y = 1|X), the probability of Y being 1 knowing X.

Logistic Regression Model

But linear regression is also not suited for predicting probabilities, as its predicted values are principially unbounded.

Use a trick and transform the unbounded target by a function that forces it into the unit interval [0, 1], e.g., the logistic function.

Logistic regression model:

$$p(Y = 1 \mid X) = \text{logistic}(\langle X, \beta \rangle) + \epsilon = \frac{e^{\sum_{i=1}^{n} \beta_i X_i}}{1 + e^{\sum_{i=1}^{n} \beta_i X_i}} + \epsilon$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 8/40

Machine Learning / 2. Logistic Regression

A Naive Estimator

A naive estimator could fit the linear regression model to Y (treated as continous target) directly, i.e.,

$$Y = \langle X, \beta \rangle + \epsilon$$

and then post-process the linear prediction via

$$\hat{p}(Y=1 \mid X) = \operatorname{logistic}(\hat{Y}) = \operatorname{logistic}(\langle X, \hat{\beta} \rangle) = \frac{e^{\sum_{i=1}^{n} \beta_i X_i}}{1 + e^{\sum_{i=1}^{n} \hat{\beta}_i X_i}}$$

But

- $\hat{\beta}$ have the property to give minimal RSS for \hat{Y} , but what properties do the $\hat{p}(Y = 1 | X)$ have?
- A probabilistic interpretation requires normal errors for *Y*, which is not adequate as *Y* is bounded to [0, 1].





Maximum Likelihood Estimator

Sound Street Str

As fit criterium, again the likelihood is used.

As Y is binary, it has a Bernoulli distribution:

 $Y|X = \mathsf{Bernoulli}(p(Y = 1 \,|\, X))$

Thus, the conditional likelihood function is:

$$\begin{split} L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta}) &= \prod_{i=1}^{n} p(Y = y_i \,|\, X = x_i; \hat{\beta}) \\ &= \prod_{i=1}^{n} p(Y = 1 \,|\, X = x_i; \hat{\beta})^{y_i} (1 - p(Y = 1 \,|\, X = x_i; \hat{\beta}))^{1 - y_i} \end{split}$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 10/40

Machine Learning / 2. Logistic Regression

Background: Gradient Descent

Given a function $f : \mathbb{R}^n \to \mathbb{R}$, find x with minimal f(x).

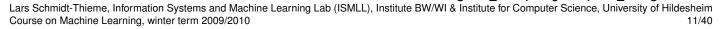
Idea: start from a random x_0 and then improve step by step, i.e., choose x_{n+1} with

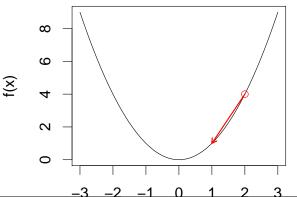
$$f(x_{n+1}) \le f(x_n)$$

Choose the negative gradient $-\frac{\partial f}{\partial x}(x_n)$ as direction for descent, i.e.,

$$x_{n+1} - x_n = -\alpha_n \cdot \frac{\partial f}{\partial x}(x_n)$$

with a suitable step length $\alpha_n > 0$.







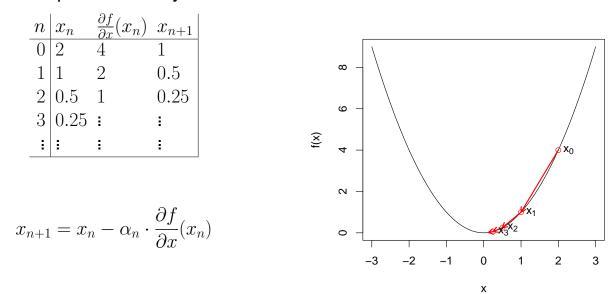
Background: Gradient Descent / Example

Example:

$$f(x) := x^2, \quad \frac{\partial f}{\partial x}(x) = 2x, \quad x_0 := 2, \quad \alpha_n :\equiv 0.25$$

Then we compute iteratively:

using



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 12/40

Machine Learning / 2. Logistic Regression

Background: Gradient Descent / Step Length

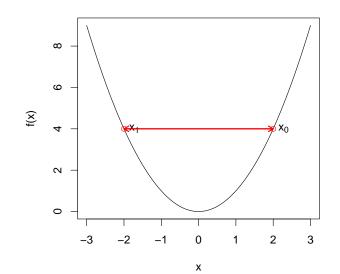
2003

Why do we need a step length? Can we set $\alpha_n \equiv 1$?

The negative gradient gives a direction of descent only in

The negative gradient gives a direction of descent only in an infinitesimal neighborhood of x_n .

Thus, the step length may be too large, and the function value of the next point does not decrease.



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 13/40



Background: Gradient Descent / Step Length

There are many different strategies to adapt the step length s.t.

- 1. the function value actually decreases and
- 2. the step length becomes not too small (and thus convergence slow)

Armijo-Principle:

$$\alpha_n := \max\{\alpha \in \{2^{-j} \mid j \in \mathbb{N}_0\} \mid f(x_n - \alpha \frac{\partial f}{\partial x}(x_n)) \le f(x_n) - \alpha \delta \langle \frac{\partial f}{\partial x}(x_n), \frac{\partial f}{\partial x}(x_n) \rangle \}$$

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

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 14/40

Machine Learning / 2. Logistic Regression

Background: Newton Algorithm

Given a function $f : \mathbb{R}^n \to \mathbb{R}$, find x with minimal f(x).

The Newton algorithm is based on a quadratic Taylor expansion of f around x_n :

$$F_n(x) := f(x_n) + \left\langle \frac{\partial f}{\partial x}(x_n), x - x_n \right\rangle + \frac{1}{2} \left\langle x - x_n, \frac{\partial^2 f}{\partial x \partial x^T}(x_n)(x - x_n) \right\rangle$$

and minimizes this approximation in each step, i.e.,

$$\frac{\partial F_n}{\partial x}(x_{n+1}) \stackrel{!}{=} 0$$

with

$$\frac{\partial F_n}{\partial x}(x) = \frac{\partial f}{\partial x}(x_n) + \frac{\partial^2 f}{\partial x \partial x^T}(x_n)(x - x_n)$$

which leads to the Newton algorithm:

$$\frac{\partial^2 f}{\partial x \partial x^T}(x_n)(x_{n+1} - x_n) = -\frac{\partial f}{\partial x}(x_n)$$

starting with a random x_0 and applying some control of the step length.





Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 15/40

Newton Algorithm for the Loglikelihood



$$\begin{split} L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta}) &= \prod_{i=1}^{n} p(Y=1 \mid X=x_{i}; \hat{\beta})^{y_{i}} (1-p(Y=1 \mid X=x_{i}; \hat{\beta}))^{1-y_{i}} \\ \log L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta}) &= \sum_{i=1}^{n} y_{i} \log p(Y=1 \mid X=x_{i}; \hat{\beta}) + (1-y_{i}) \log(1-p(Y=1 \mid X=x_{i}; \hat{\beta})) \\ &= \sum_{i=1}^{n} y_{i} \log(\frac{e^{\langle x_{i}, \hat{\beta} \rangle}}{1+e^{\langle x_{i}, \hat{\beta} \rangle}}) + (1-y_{i}) \log(1-\frac{e^{\langle x_{i}, \hat{\beta} \rangle}}{1+e^{\langle x_{i}, \hat{\beta} \rangle}}) \\ &= \sum_{i=1}^{n} y_{i} (\langle x_{i}, \hat{\beta} \rangle - \log(1+e^{\langle x_{i}, \hat{\beta} \rangle})) + (1-y_{i}) \log(\frac{1}{1+e^{\langle x_{i}, \hat{\beta} \rangle}}) \\ &= \sum_{i=1}^{n} y_{i} (\langle x_{i}, \hat{\beta} \rangle - \log(1+e^{\langle x_{i}, \hat{\beta} \rangle})) + (1-y_{i})(-\log(1+e^{\langle x_{i}, \hat{\beta} \rangle})) \\ &= \sum_{i=1}^{n} y_{i} \langle x_{i}, \hat{\beta} \rangle - \log(1+e^{\langle x_{i}, \hat{\beta} \rangle}) \end{split}$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 16/40

Machine Learning / 2. Logistic Regression

Newton Algorithm for the Loglikelihood



$$\log L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta}) = \sum_{i=1}^{n} y_i \langle x_i, \hat{\beta} \rangle - \log(1 + e^{\langle x_i, \hat{\beta} \rangle})$$
$$\frac{\partial L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta})}{\partial \hat{\beta}} = \sum_{i=1}^{n} y_i x_i - \frac{1}{1 + e^{\langle x_i, \hat{\beta} \rangle}} e^{\langle x_i, \hat{\beta} \rangle} x_i$$
$$= \sum_{i=1}^{n} x_i (y_i - p(Y = 1 \mid X = x_i; \hat{\beta}))$$
$$= \mathbf{X}^T (\mathbf{y} - \mathbf{p})$$

with

$$\mathbf{p} := \begin{pmatrix} p(Y=1 \mid X=x_1; \hat{\beta})) \\ \vdots \\ p(Y=1 \mid X=x_n; \hat{\beta})) \end{pmatrix}$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 17/40

Newton Algorithm for the Loglikelihood

$$\begin{aligned} \frac{\partial L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta})}{\partial \hat{\beta}} = \mathbf{X}^{T}(\mathbf{y} - \mathbf{p}) \\ \frac{\partial^{2} L_{\mathcal{D}}^{\mathsf{cond}}(\hat{\beta})}{\partial \hat{\beta} \partial \hat{\beta}^{T}} = \sum_{i=1}^{n} -x_{i} p(Y = 1 \mid X = x_{i}; \hat{\beta})(1 - p(Y = 1 \mid X = x_{i}; \hat{\beta}))x_{i}^{T} \\ = -\sum_{i=1}^{n} x_{i} x_{i}^{T} p(Y = 1 \mid X = x_{i}; \hat{\beta})(1 - p(Y = 1 \mid X = x_{i}; \hat{\beta})) \\ = -\mathbf{X}^{T} \mathbf{W} \mathbf{X} \end{aligned}$$

with

$$\mathbf{W} := \begin{pmatrix} q(x_1; \hat{\beta})(1 - q(x_1; \hat{\beta})) & 0 & \dots & 0 \\ 0 & \ddots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & q(x_n; \hat{\beta})(1 - q(x_n; \hat{\beta})) \end{pmatrix}$$

and $q(x; \hat{\beta}) := P(Y = 1 | X = x; \hat{\beta}).$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 18/40

Machine Learning / 2. Logistic Regression

Newton Algorithm for the Loglikelihood

Newton algorithm:

$$\frac{\partial^2 \log L}{\partial \hat{\beta} \partial \hat{\beta}^T} (\hat{\beta}_n) (\hat{\beta}_{n+1} - \hat{\beta}_n) = -\frac{\partial \log L}{\partial \hat{\beta}} (\hat{\beta}_n) - \mathbf{X}^T \mathbf{W} \mathbf{X} (\hat{\beta}_{n+1} - \hat{\beta}_n) = -\mathbf{X}^T (\mathbf{y} - \mathbf{p})$$

$$\mathbf{X}^T \mathbf{W} \mathbf{X} \hat{\beta}_{n+1} = \mathbf{X}^T \mathbf{W} (\mathbf{X} \hat{\beta}_n + \mathbf{W}^{-1} (\mathbf{y} - \mathbf{p}))$$

Equivalent to a weighted least squares of the "adjusted response"

$$z := \mathbf{X}\hat{\beta}_n + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p})$$

on X known as iteratively reweighted least squares (IRLS).

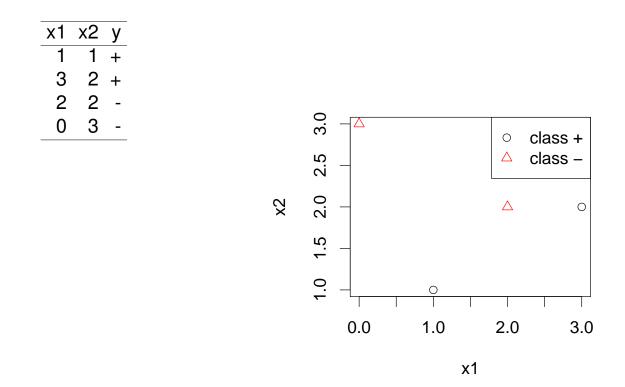
IRLS typically is started at $\hat{\beta}^{(0)} := 0$ and uses constant step length 1.



rsitär

2003

Learn a classification function for the following data:



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 20/40

Machine Learning / 2. Logistic Regression

1

Example

$$\frac{\begin{array}{cccc}
x1 & x2 & y \\
\hline 1 & 1 & + \\
3 & 2 & + , \\
2 & 2 & - \\
\hline 0 & 3 & -
\end{array}} \mathbf{X} := \begin{pmatrix} 1 & 1 & 1 \\
1 & 3 & 2 \\
1 & 2 & 2 \\
1 & 0 & 3 \end{pmatrix}, \quad \mathbf{y} := \begin{pmatrix} 1 \\
1 \\
0 \\
0 \\
0 \end{pmatrix}, \quad \hat{\beta}^{(0)} := \begin{pmatrix} 0 \\
0 \\
0 \\
0 \\
0 \\
\end{array}$$

$$\mathbf{p}^{(0)} := \left(\frac{e^{\langle \beta, x_i \rangle}}{1 + e^{\langle \beta, x_i \rangle}}\right)_i = \begin{pmatrix} 0.5\\0.5\\0.5\\0.5 \end{pmatrix}, \quad w^{(0)} := \mathbf{p}^{(0)}(1 - \mathbf{p}^{(0)}) = \begin{pmatrix} 0.25\\0.25\\0.25\\0.25 \end{pmatrix},$$
$$z^{(0)} := \mathbf{X}\hat{\beta}^{(0)} + \mathbf{W}^{(0)^{-1}}(\mathbf{y} - \mathbf{p}^{(0)}) = \begin{pmatrix} 2\\2\\-2\\-2\\-2 \end{pmatrix}$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 21/40

Visualization Logistic Regression Models

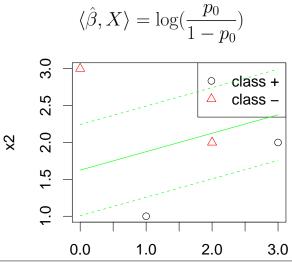
To visualize a logistic regression model, we can plot the decision boundary

$$\hat{p}(Y = 1 \mid X) = \frac{1}{2}$$

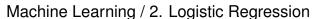
and more detailed some level lines

$$\hat{p}(Y=1 \mid X) = p_0$$

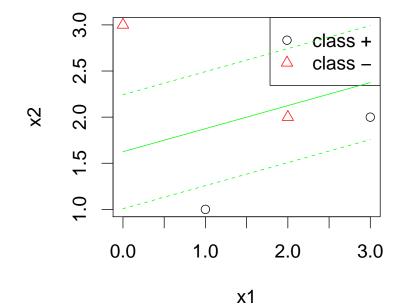
e.g., for $p_0 = 0.25$ and $p_0 = 0.75$:



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 x1 22/40



Example

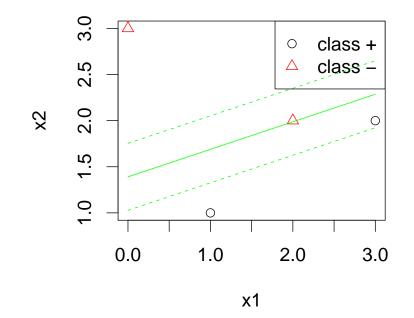


Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40

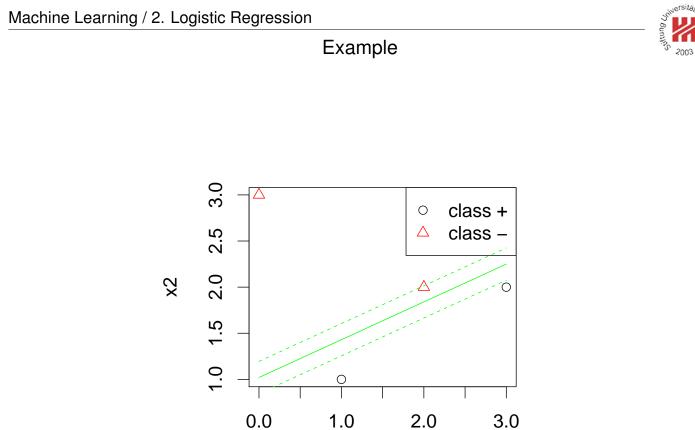








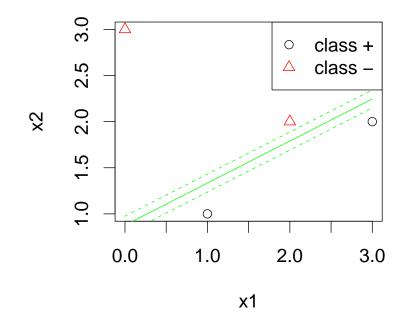
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40



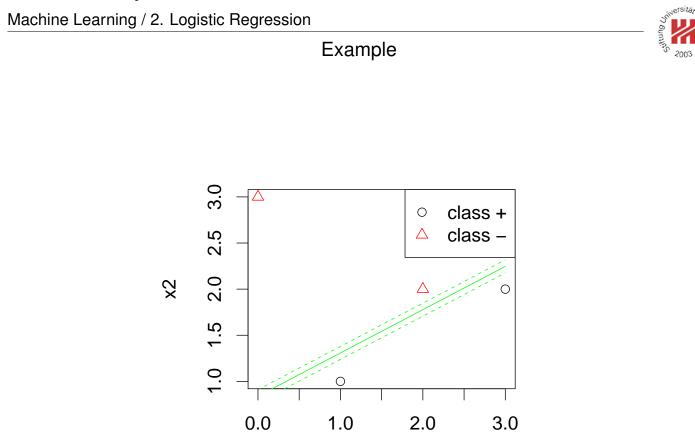
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40

x1





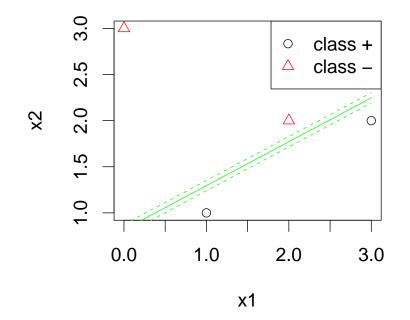
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40



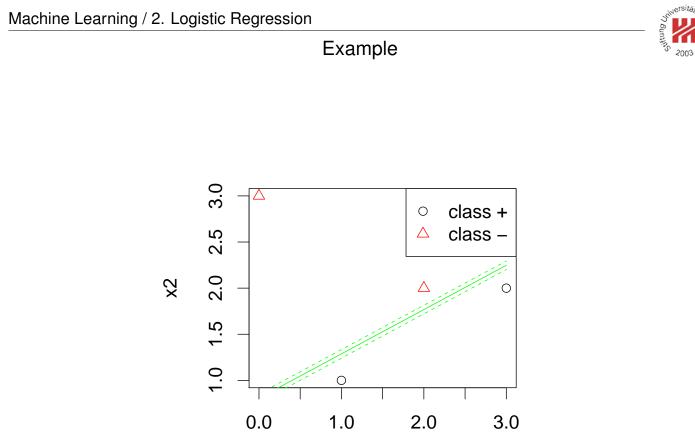
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40

x1





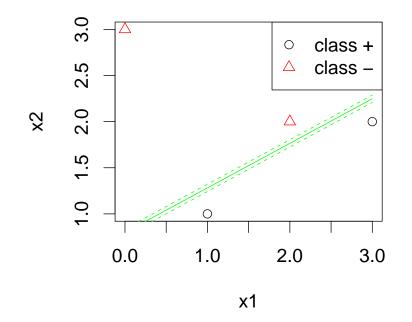
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40



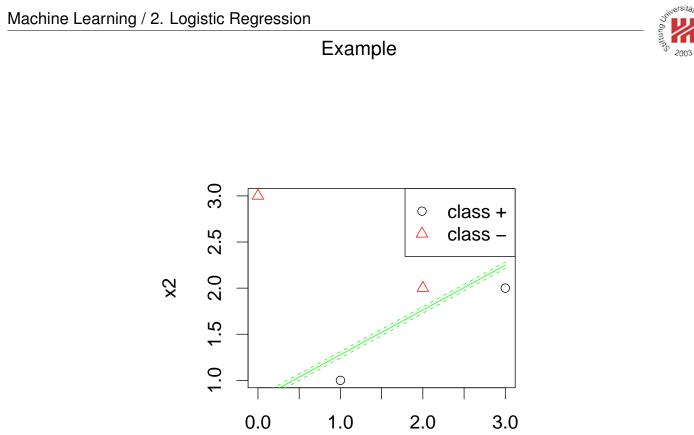
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40

x1



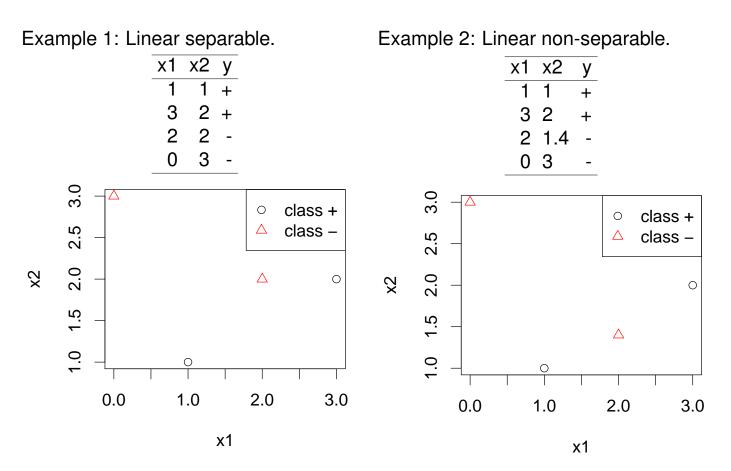


Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40

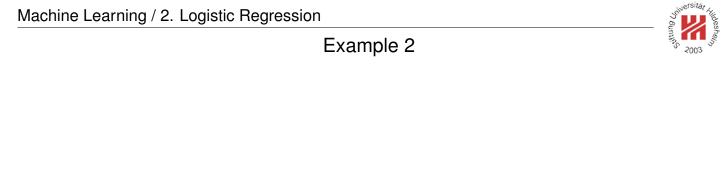


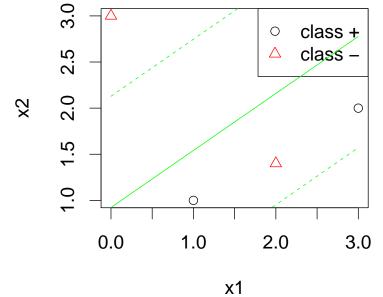
Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 23/40

Linear separable vs. linear non-separable



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 24/40

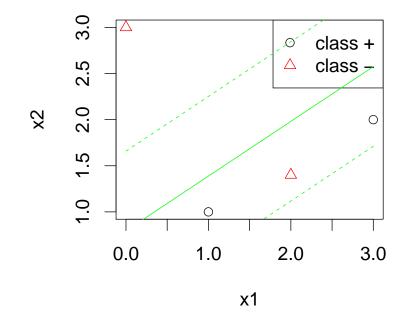




Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 25/40



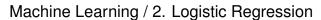


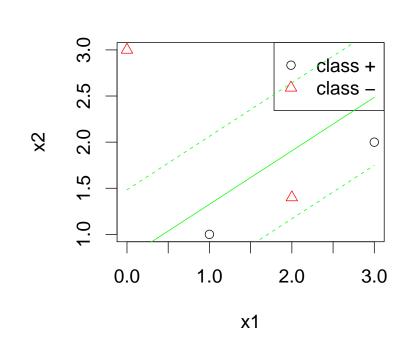


Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 25/40

Example 2



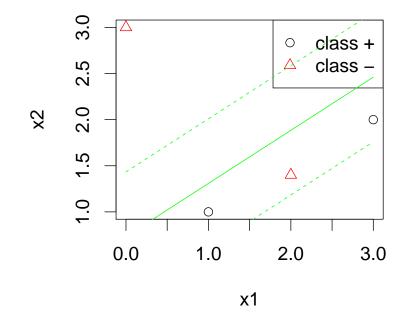




Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 25/40







Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 25/40

Machine Learning



1. The Classification Problem

- 2. Logistic Regression
- **3. Multi-category Targets**
- 4. Linear Discriminant Analysis

Binary vs. Multi-category Targets



Binary Targets / Binary Classification:

prediction of a nominal target variable with 2 levels/values.

Example: spam vs. non-spam.

Multi-category Targets / Multi-class Targets / Polychotomous Classification:

prediction of a nominal target variable with more than 2 levels/values.

Example: three iris species; 10 digits; 26 letters etc.

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 26/40

Machine Learning / 3. Multi-category Targets

Compound vs. Monolithic Classifiers

Compound models

- built from binary submodels,
- different types of compound models employ different sets of submodels:

1-vs-rest (aka 1-vs-all) 1-vs-last

1-vs-1 (Dietterich and Bakiri 1995; aka pairwise classification) **DAG**

- using error-correcting codes to combine component models.
- also ensembles of compound models are used (Frank and Kramer 2004).

Monolithic models (aka "'one machine"' (Rifkin and Klautau 2004))

- trying to solve the multi-class target problem intrinsically
- examples: decision trees, special SVMs, etc.



Types of Compound Models

1-vs-rest: one binary classifier per class:

$$f_y : X \to [0, 1], \quad y \in Y$$
$$f(x) := \left(\frac{f_1(x)}{\sum_{y \in Y} f_y(x)}, \dots, \frac{f_k(x)}{\sum_{y \in Y} f_y(x)}\right)$$

1-vs-last: one binary classifier per class (but last y_k):

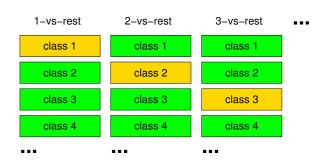
$$f(x) := \left(\frac{f_1(x)}{1 + \sum_{y \in Y} f_y(x)}, \dots, \frac{f_y : X \to [0, 1], \quad y \in Y, y \neq y_k}{1 + \sum_{y \in Y} f_y(x)}, \frac{f_{k-1}(x)}{1 + \sum_{y \in Y} f_y(x)}, \frac{1}{1 + \sum_{y \in Y} f_y(x)}\right)$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 28/40

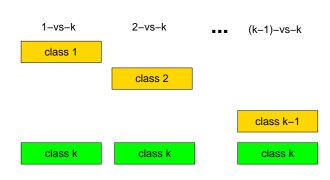
Machine Learning / 3. Multi-category Targets

Polychotomous Discrimination, k target categories

1-vs-rest construction:



1-vs-last construction:



\boldsymbol{k} classifiers trained on \boldsymbol{N} cases

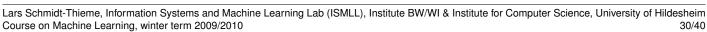
kN cases in total

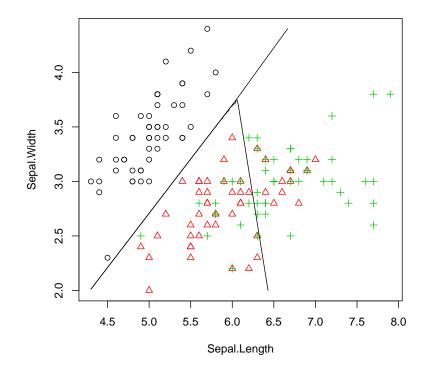
k-1 classifiers trained on approx. 2 N/k on average.

 $N + (k-2)N_k$ cases in total

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 29/40

Example / Iris data / Logistic Regression

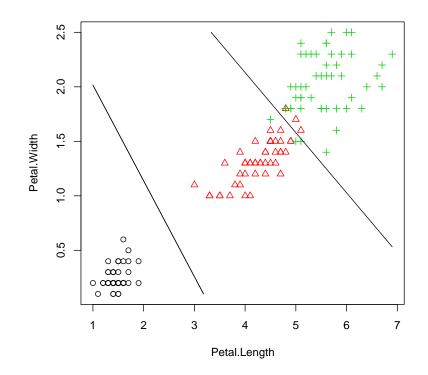




Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 30/40

Machine Learning / 3. Multi-category Targets

Example / Iris data / Logistic Regression









- 1. The Classification Problem
- 2. Logistic Regression
- 3. Multi-category Targets
- 4. Linear Discriminant Analysis

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 31/40

Machine Learning / 4. Linear Discriminant Analysis

Assumptions



In discriminant analysis, it is assumed that

• cases of a each class *k* are generated according to some probabilities

$$\pi_k = p(Y = k)$$

and

• its predictor variables are generated by a class-specific multivariate normal distribution

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma_k)$$

i.e.

$$p_k(x) := \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma_k|^{\frac{1}{2}}} e^{-\frac{1}{2} \langle x - \mu_k, \Sigma^{-1}(x - \mu_k) \rangle}$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 31/40

Decision Rule

Discriminant analysis predicts as follows:

$$\hat{Y}|X = x := \operatorname{argmax}_k \pi_k p_k(x) = \operatorname{argmax}_k \delta_k(x)$$

with the discriminant functions

$$\delta_k(x) := -\frac{1}{2} \log |\Sigma_k| - \frac{1}{2} \langle x - \mu_k, \Sigma_k^{-1}(x - \mu_k) \rangle + \log \pi_k$$

Here,

$$\langle x - \mu_k, \Sigma_k^{-1}(x - \mu_k) \rangle$$

is called the Mahalanobis distance of x and μ_k .

Thus, discriminant analysis can be described as **prototype method**, where

- each class k is represented by a prototype μ_k and
- cases are assigned the class with the nearest prototype.

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 32/40

Machine Learning / 4. Linear Discriminant Analysis

Maximum Likelihood Parameter Estimates

The maximum likelihood parameter estimates are as follows:

$$\hat{n}_k := \sum_{i=1}^n I(y_i = k), \quad \text{with } I(x = y) := \begin{cases} 1, \text{ if } x = y \\ 0, \text{ else} \end{cases}$$
$$\hat{\pi}_k := \frac{\hat{n}_k}{n}$$
$$\hat{\mu}_k := \frac{1}{\hat{n}_k} \sum_{i:y_i = k} x_i$$
$$\hat{\Sigma}_k := \frac{1}{\hat{n}_k} \sum_{i:y_i = k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$





QDA vs. LDA

In the general case, decision boundaries are quadratic due to the quadratic occurrence of x in the Mahalanobis distance. This is called **quadratic discriminant analysis (QDA)**.

If we assume that all classes share the same covariance matrix, i.e.,

$$\Sigma_k = \Sigma_{k'} \quad \forall k, k'$$

then this quadratic term is canceled and the decision boundaries become linear. This model is called **linear discriminant analysis (LDA)**.

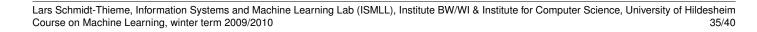
The maximum likelihood estimator for the common covariance matrix in LDA is

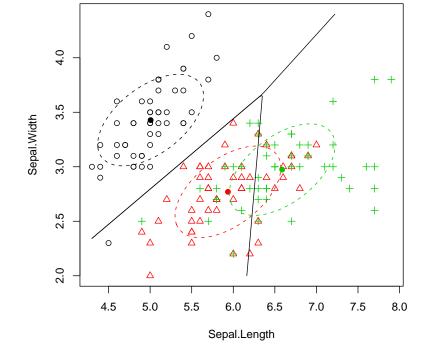
$$\hat{\Sigma} := \sum_k \frac{\hat{n}_k}{n} \hat{\Sigma}_k$$

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 34/40

Machine Learning / 4. Linear Discriminant Analysis









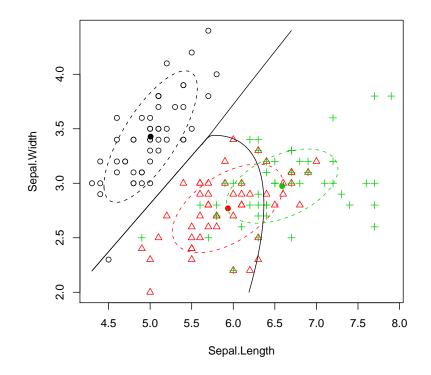


Example / Iris data / QDA



sitä

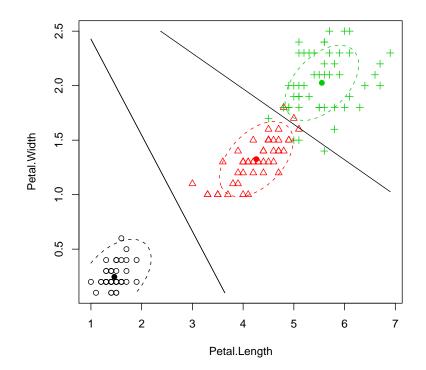
2003



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 35/40



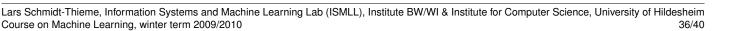




Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 35/40 Course on Machine Learning, winter term 2009/2010

Machine Learning / 4. Linear Discriminant Analysis

Example / Iris data / QDA



The variance matrix estimated by LDA can be used to linearly transform the data s.t. the Mahalanobis distance

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim

LDA coordinates

$$\langle x, \hat{\Sigma}^{-1}y \rangle = x^T \hat{\Sigma}^{-1}y$$

becomes the standard euclidean distance in the transformed coordinates

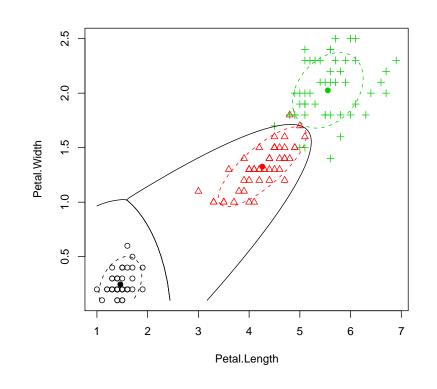
$$\langle x', y' \rangle = x^T y$$

This is accomplished by decomposing $\hat{\Sigma}$ as

$$\hat{\Sigma} = U D U^T$$

with an orthonormal matrix U (i.e., $U^T = U^{-1}$) and a diagonal matrix D and setting

$$x' := D^{-\frac{1}{2}} U^T x$$







Course on Machine Learning, winter term 2009/2010

model.

Machine Learning / 4. Linear Discriminant Analysis

Example / Iris data / LDA coordinates



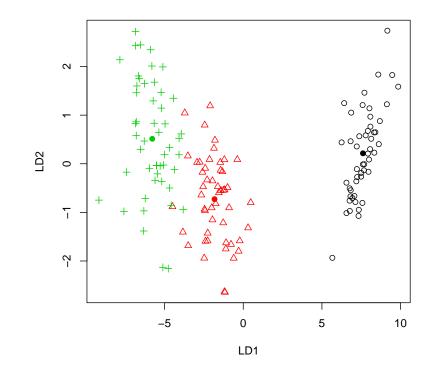


LDA and logistic regression use the same underlying linear

$$\log(\frac{P(Y=1|X=x)}{P(Y=0|X=x)}) = \log(\frac{\pi_1}{\pi_0}) - \frac{1}{2}\langle\mu_0 + \mu_1, \Sigma^{-1}(\mu_1 - \mu_0)\rangle + \langle x, \Sigma^{-1}(\mu_1 - \mu_0)\rangle = \alpha_0 + \langle \alpha, x \rangle$$

For logistic regression by definition we have:

$$\log(\frac{P(Y=1|X=x)}{P(Y=0|X=x)}) = \beta_0 + \langle \beta, x \rangle$$



Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim

LDA vs. Logistic Regression





37/40

LDA vs. Logistic Regression



Both models differ in the way they estimate the parameters.

LDA maximizes the **complete likelihood**:

$$\prod_{i} p(x_{i}, y_{i}) = \underbrace{\prod_{i} p(x_{i} \mid y_{i})}_{\text{normal } p_{k}} \underbrace{\prod_{i} p(y_{i})}_{\text{bernoulli } \pi_{k}}$$

While logistic regression maximizes the **conditional likelihood** only:

$\prod p(x_i, y_i) =$	$\prod p(y_i x_i)$	$\prod f(x_i)$
i		ignored

Lars Schmidt-Thieme, Information Systems and Machine Learning Lab (ISMLL), Institute BW/WI & Institute for Computer Science, University of Hildesheim Course on Machine Learning, winter term 2009/2010 39/40

Machine Learning / 4. Linear Discriminant Analysis

Summary

- For classification, **logistic regression models** of type $Y = \frac{e^{\langle X,\beta \rangle}}{1+e^{\langle X,\beta \rangle}} + \epsilon$ can be used to predict a binary *Y* based on several (quantitative) *X*.
- The maximum likelihood estimates (MLE) have to be computed using Newton's algorithm on the loglikelihood. The resulting procedure can be reinterpreted as iteratively reweighted least squares (IRLS).
- Another simple classification model is linear discriminant analysis
 (LDA) that assumes that the cases of each class have been generated by a multivariate normal distribution with class-specific means μ_k (the class prototype) and a common covariance matrix Σ.
- The maximum likelihood parameter estimates $\hat{\pi}_k$, $\hat{\mu}_k$, $\hat{\Sigma}$ for LDA are just the sample estimates.
- Logistic regression and LDA share the same underlying linear model, but logistic regression optimizes the **conditional likelihood**, LDA the **complete likelihood**.