Machine Learning

A. Supervised Learning: Linear Models & Fundamentals

A.2. Linear Classification

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Syllabus

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1. The Classification Problem
2. Logistic Regression
3. Logistic Regression via Gradient Ascent
4. Logistic Regression via Newton
5. Multi-category Targets
6. Linear Discriminant Analysis

Outline

The Classification Problem

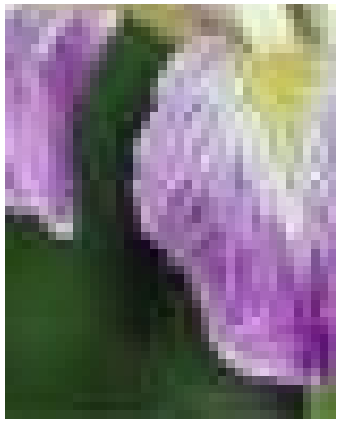
Example: classifying iris plants (Anderson 1935).

iris setosa

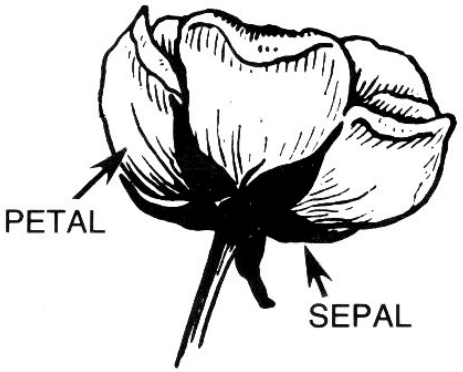
iris versicolor

150 iris plants (50 of each species):

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



iris virginica



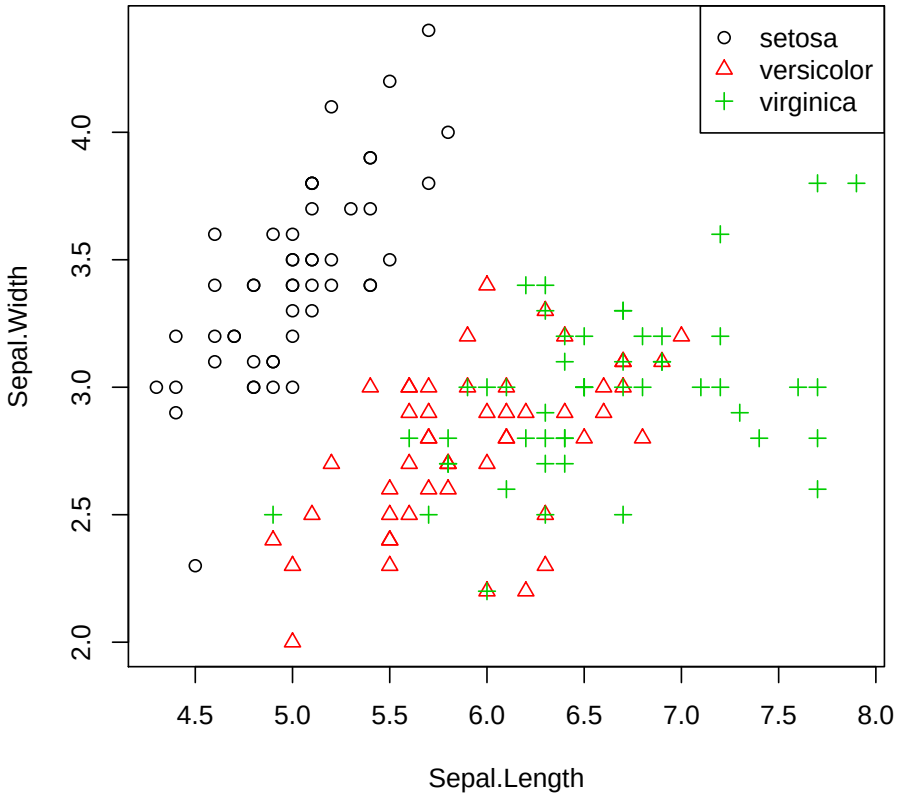
Given the lengths and widths of sepals and petals of an instance, which iris species does it belong to?

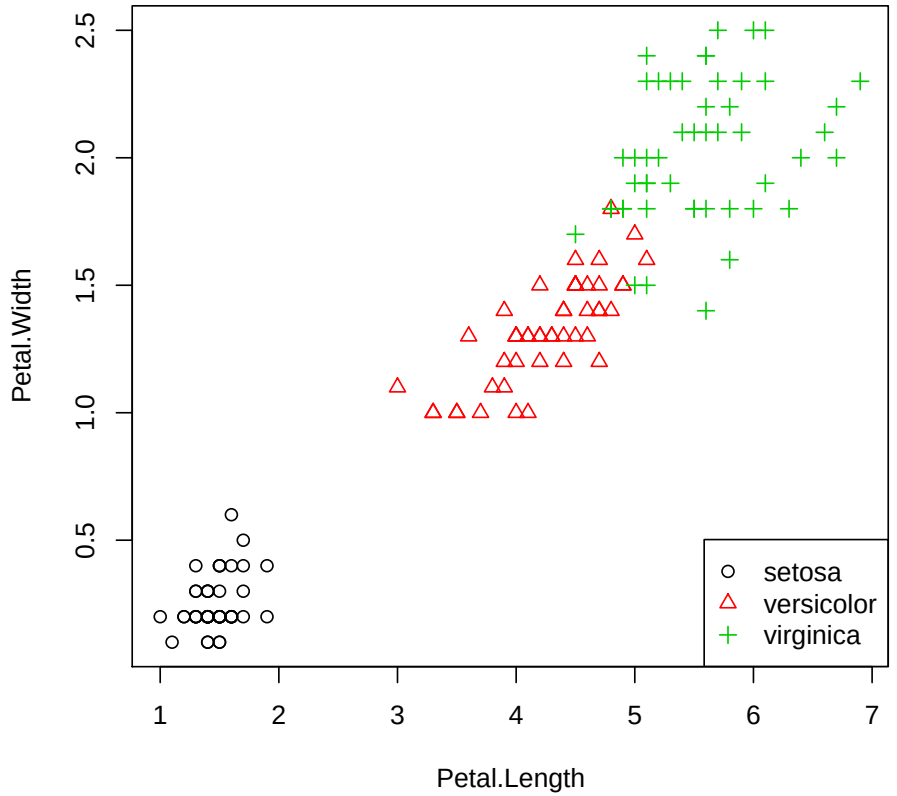
[source: iris species database, http://www.badbear.com/signa]

The Classification Problem / Data

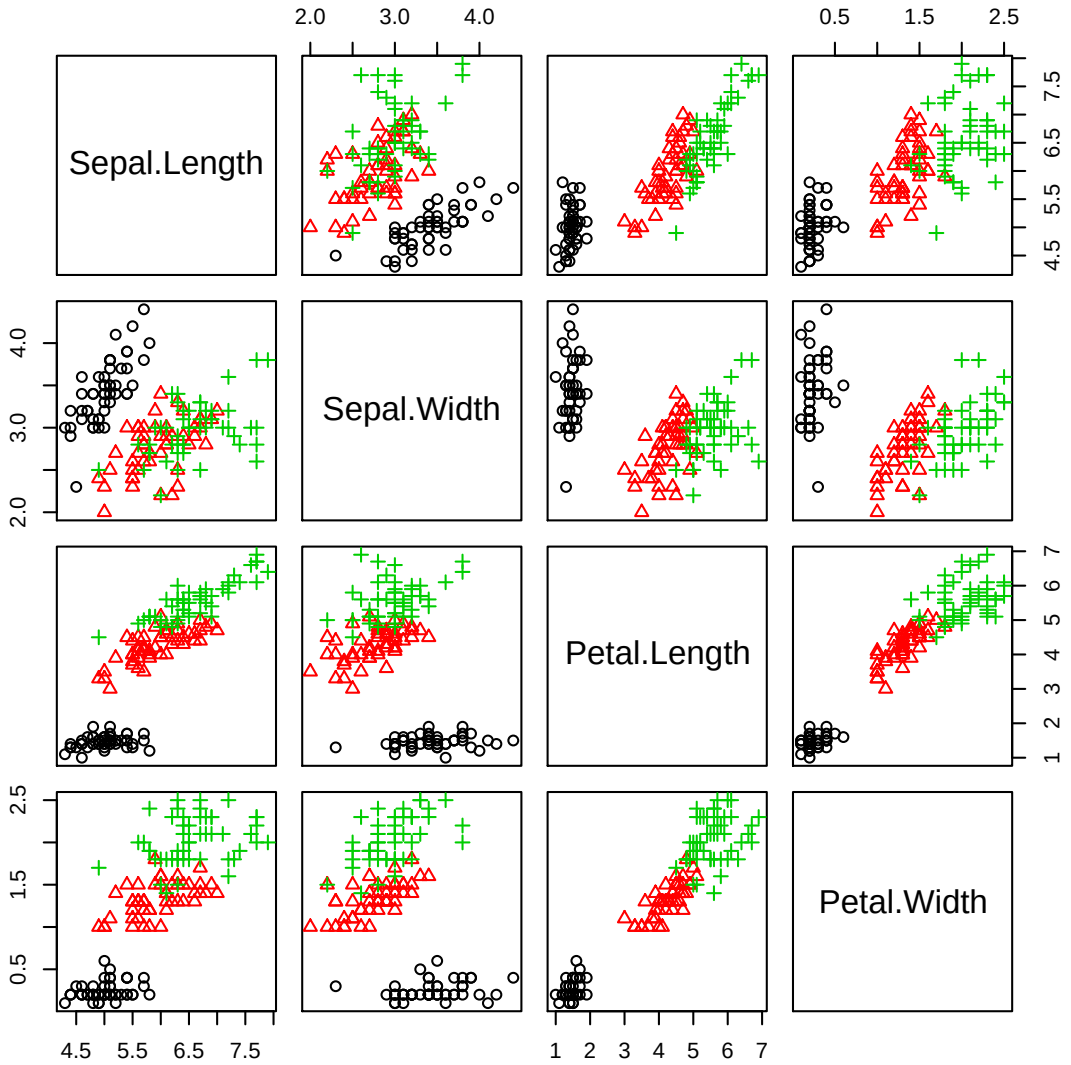
	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.10	3.50	1.40	0.20	setosa
2	4.90	3.00	1.40	0.20	setosa
3	4.70	3.20	1.30	0.20	setosa
⋮	⋮	⋮	⋮	⋮	
51	7.00	3.20	4.70	1.40	versicolor
52	6.40	3.20	4.50	1.50	versicolor
53	6.90	3.10	4.90	1.50	versicolor
⋮	⋮	⋮	⋮	⋮	
101	6.30	3.30	6.00	2.50	virginica
⋮	⋮	⋮	⋮	⋮	
150	5.90	3.00	5.10	1.80	virginica

The Classification Problem





The Classification Problem



Binary Classification

Let us start simple and consider two classes only,
e.g., target space $\mathcal{Y} := \{0, 1\}$.

Given

- a set $\mathcal{D}^{\text{train}} := \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\} \subseteq \mathbb{R}^M \times \mathcal{Y}$ called **training data**,

we want to estimate a model $\hat{y}(x)$ s.t. for a set $\mathcal{D}^{\text{test}} \subseteq \mathbb{R}^M \times \mathcal{Y}$ called **test set** the **test error** (here: **misclassification rate**)

$$\text{err}(\hat{y}; \mathcal{D}^{\text{test}}) := \text{mcr}(\hat{y}; \mathcal{D}^{\text{test}}) := \frac{1}{|D^{\text{test}}|} \sum_{(x,y) \in \mathcal{D}^{\text{test}}} I(y \neq \hat{y}(x))$$

is minimal.

Note: $I(A) := 1$ if statement A is true, $I(A) := 0$ otherwise (**indicator function**).
$\mathcal{D}^{\text{test}}$ has (i) to be from the same data generating process and (ii) not to be available during training.

Binary Classification / Data

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species setosa
1	5.10	3.50	1.40	0.20	1
2	4.90	3.00	1.40	0.20	1
3	4.70	3.20	1.30	0.20	1
⋮	⋮	⋮	⋮	⋮	
51	7.00	3.20	4.70	1.40	0
52	6.40	3.20	4.50	1.50	0
53	6.90	3.10	4.90	1.50	0
⋮	⋮	⋮	⋮	⋮	
101	6.30	3.30	6.00	2.50	0
⋮	⋮	⋮	⋮	⋮	
150	5.90	3.00	5.10	1.80	0

Outline

Binary Classification with Linear Regression

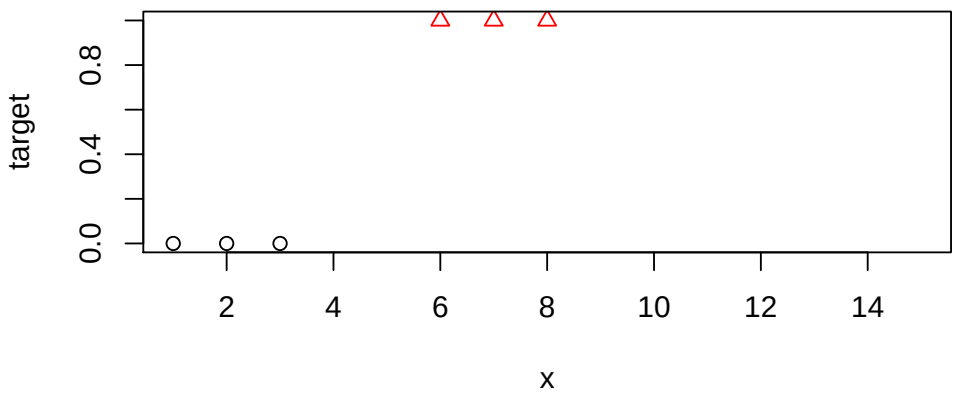
One idea could be to optimize the linear regression model

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

for RSS.

This has several problems

- It is not suited for predicting y as it can assume all kinds of intermediate values.
- It is optimizing for the wrong loss.



Binary Classification with Linear Regression

Instead of predicting Y directly, we predict

$p(Y = 1|X;\ \beta)$ — the probability of Y being 1 knowing X.

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

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

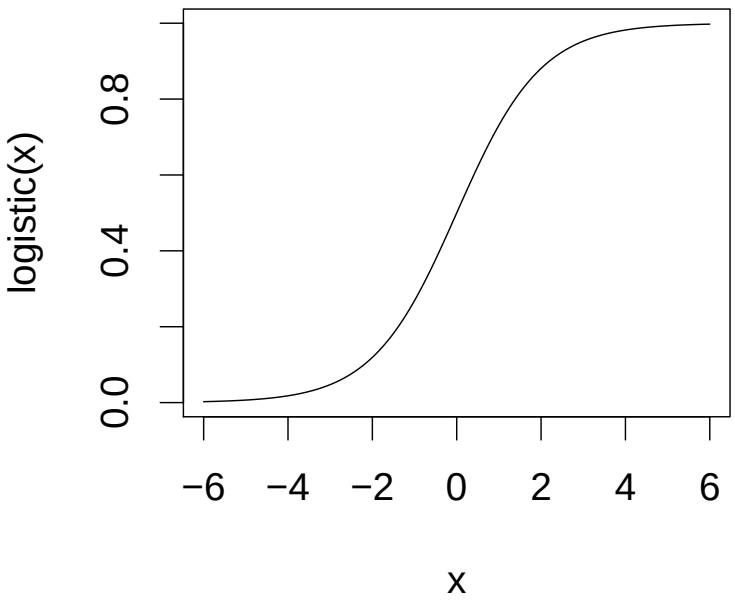
Logistic Function

Logistic function:

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

Basic properties:

- has values between 0 and 1,
- converges to 1 when approaching $+\infty$,
- converges to 0 when approaching $-\infty$,
- is smooth and symmetric at $(0, 0.5)$.



Logistic Regression Model

$$p(Y = 1 \mid X;\ \beta) = \text{logistic}(\langle X, \beta \rangle) + \epsilon = \frac{e^{\sum_{m=1}^{M} \beta_m x_m}}{1 + e^{\sum_{m=1}^{M} \beta_m x_m}} + \epsilon$$

- observed targets are converted to probabilities $0, 1$
  - probability 1 for targets $Y = 1$,
    probability 0 for targets $Y = 0$
  - ϵ is a random variable called **noise**
- predicted targets are probabilities $[0, 1]$

$$\hat{y}(x;\ \hat{\beta}) := \text{logistic}(\langle x, \hat{\beta} \rangle) = \frac{e^{\sum_{m=1}^{M} \hat{\beta}_m x_m}}{1 + e^{\sum_{m=1}^{M} \hat{\beta}_m x_m}}$$

- remember: a logistic regression model is a **classification model**
  - despite its name

Loss Function

Misclassification rate

$$\begin{aligned}\mathrm{mcr}(\hat{\beta}; \mathcal{D}^{\mathrm{test}}) &:= \mathrm{mcr}(\hat{y}(.; \hat{\beta}); \mathcal{D}^{\mathrm{test}}) \\ &= \frac{1}{|D^{\mathrm{test}}|} \sum_{(x,y) \in \mathcal{D}^{\mathrm{test}}} I(y \neq \hat{y}(x; \hat{\beta})) \\ &= \frac{1}{|D^{\mathrm{test}}|} \sum_{(x,y) \in \mathcal{D}^{\mathrm{test}}} I(y \neq I(\mathrm{logistic}(\hat{\beta}^T x) \geq 0.5))\end{aligned}$$

Loss Function

Misclassification rate

$$\begin{aligned}\mathrm{mcr}(\hat{\beta}; \mathcal{D}^{\mathrm{test}}) &:= \mathrm{mcr}(\hat{y}(.;\hat{\beta}); \mathcal{D}^{\mathrm{test}}) \\ &= \frac{1}{|D^{\mathrm{test}}|} \sum_{(x,y)\in\mathcal{D}^{\mathrm{test}}} I(y \neq \hat{y}(x;\hat{\beta})) \\ &= \frac{1}{|D^{\mathrm{test}}|} \sum_{(x,y)\in\mathcal{D}^{\mathrm{test}}} I(y \neq I(\mathrm{logistic}(\hat{\beta}^T x) \geq 0.5))\end{aligned}$$

is unsuited as loss function for minimization as it is not continuous.

Use a continuous **proxy loss** instead, e.g., adhoc

$$\begin{aligned}\ell(\hat{y}; \mathcal{D}^{\mathrm{test}})) = \frac{1}{|D^{\mathrm{test}}|} \sum_{(x,y)\in\mathcal{D}^{\mathrm{test}}} & I(y=0)\ \mathrm{logistic}(\hat{\beta}^T x) \\ & + I(y=1)\ (1 - \mathrm{logistic}(\hat{\beta}^T x))\end{aligned}$$

Maximum Likelihood Estimator

As fit criterium, the likelihood is used.

As Y is binary, it has a Bernoulli distribution:

$$Y|X = \text{Bernoulli}(p(Y = 1 \mid X))$$

Thus, the conditional likelihood function is:

$$\begin{aligned} L_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) &= \prod_{n=1}^{N} p(Y = y_n \mid X = x_n; \hat{\beta}) \\ &= \prod_{n=1}^{N} p(Y = 1 \mid X = x_n; \hat{\beta})^{y_n} (1 - p(Y = 1 \mid X = x_n; \hat{\beta}))^{1-y_n} \end{aligned}$$

Estimating Model Parameters

The last step is to estimate the model parameters $\hat{\beta}$.

This will be done by

- maximizing the **conditional likelihood function** $L_{\mathcal{D}}^{\mathbf{cond}}$ which is equivalent to
- maximizing the **log likelihood** $log(L_{\mathcal{D}}^{\mathbf{cond}})$

This can be done with any optimization technique. We will have a closer look at

- Gradient Ascent
  - = Gradient Descent, but for maximization: update direction is just the gradient.
- Newton Method

Outline

Gradient Ascent

maximize-GA$(f : \mathbb{R}^N \to \mathbb{R}, x_0 \in \mathbb{R}^N, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:
  for $t := 1, \ldots, t_{\max}$:
    $x^{(t)} := x^{(t-1)} + \mu \cdot \frac{\partial f}{\partial x}(x^{(t-1)})$
    if $f(x^{(t)}) - f(x^{(t-1)}) < \epsilon$:
      return $x^{(t)}$
  raise exception "not converged in $t_{\max}$ iterations"

For maximizing function f instead of minimizing it go to the positive direction of the gradient.

Gradient Ascent for the Loglikelihood

$$\log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) = \sum_{n=1}^{N} y_n \log \hat{y}_n + (1-y_n)\log(1-\hat{y}_n)$$

$$= \sum_{n=1}^{N} y_n \log\left(\frac{e^{\langle x_n,\hat{\beta}\rangle}}{1+e^{\langle x_n,\hat{\beta}\rangle}}\right) + (1-y_n)\log\left(1-\frac{e^{\langle x_n,\hat{\beta}\rangle}}{1+e^{\langle x_n,\hat{\beta}\rangle}}\right)$$

$$= \sum_{n=1}^{N} y_n(\langle x_n,\hat{\beta}\rangle - \log(1+e^{\langle x_n,\hat{\beta}\rangle})) + (1-y_n)\log\left(\frac{1}{1+e^{\langle x_n,\hat{\beta}\rangle}}\right)$$

$$= \sum_{n=1}^{N} y_n(\langle x_n,\hat{\beta}\rangle - \log(1+e^{\langle x_n,\hat{\beta}\rangle})) + (1-y_n)(-\log(1+e^{\langle x_n,\hat{\beta}\rangle}))$$

$$= \sum_{n=1}^{N} y_n\langle x_n,\hat{\beta}\rangle - \log(1+e^{\langle x_n,\hat{\beta}\rangle})$$

Gradient Ascent for the Loglikelihood

$$\log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) = \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$$

$$\nabla_\beta \log L_{\mathcal{D}}^{\text{cond}} = \frac{\partial \log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta})}{\partial \hat{\beta}} = \sum_{n=1}^{N} y_n x_n - \frac{1}{1 + e^{\langle x_n, \hat{\beta} \rangle}} e^{\langle x_n, \hat{\beta} \rangle} x_n$$

$$= \sum_{n=1}^{N} x_n (y_n - \hat{y}_n)$$

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

$$\hat{\mathbf{y}} := \begin{pmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_N \end{pmatrix}$$

Gradient Ascent for the Loglikelihood

learn-logreg-GA$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$\ell := \log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) := \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$

$\hat{\beta} :=$ maximize-GA$(\ell, 0_M, \mu, t_{\max}, \epsilon)$

return $\hat{\beta}$

Gradient Ascent for the Loglikelihood

learn-logreg-GA$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$X := (x_1, x_2, \ldots, x_N)^T$

$y := (y_1, y_2, \ldots, y_N)^T$

$\hat{\beta} := 0_M$

$\ell := \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$

for $t = 1, \ldots, t_{\max}$:

  $\hat{y} := (1/(1 + e^{-\hat{\beta}^T x_n})_{n \in 1:N}$

  $\hat{\beta} := \hat{\beta} + \mu \cdot X^T (y - \hat{y})$

  $\ell^{\text{old}} := \ell$

  $\ell := \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$

  if $\ell - \ell^{\text{old}} < \epsilon$:

    return $\hat{\beta}$

raise exception "not converged in $t_{\max}$ iterations"

Outline

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_t:

$$F_t(x) := f(x_t) + \langle \frac{\partial f}{\partial x}(x_t), x - x_t \rangle + \frac{1}{2} \langle x - x_t, \frac{\partial^2 f}{\partial x \partial x^T}(x_t)(x - x_t) \rangle$$

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

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

with

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

which leads to the Newton algorithm:

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

Newton Algorithm

Newton Algorithm

minimize-Newton$(f : \mathbb{R}^N \to \mathbb{R}, x^{(0)} \in \mathbb{R}^N, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:
  for $t := 1, \ldots, t_{\max}$:
    $g := \nabla f(x^{(t-1)})$
    $H := \nabla^2 f(x^{(t-1)})$
    $x^{(t)} := x^{(t-1)} - \mu H^{-1} g$
    if $f(x^{(t-1)}) - f(x^{(t)}) < \epsilon$:
      return $x^{(t)}$
  raise exception "not converged in $t_{\max}$ iterations"

$x^{(0)}$	start value
μ	(fixed) step length / learning rate
$t_{\max}$	maximal number of iterations
ϵ	minimum stepwise improvement

$\nabla f(x) \in \mathbb{R}^N$: gradient, $(\nabla f(x))_n = \frac{\partial}{\partial x_n} f(x)$

$\nabla^2 f(x) \in \mathbb{R}^{N \times N}$: Hessian matrix, $\nabla^2 f(x)_{n,m} = \frac{\partial^2 f}{\partial x_n \partial x_m}(x)$

Newton Algorithm for the Loglikelihood

$$\frac{\partial \log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta})}{\partial \hat{\beta}} = \mathbf{X}^T(\mathbf{y} - \hat{\mathbf{y}})$$

$$\frac{\partial^2 \log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta})}{\partial \hat{\beta} \partial \hat{\beta}^T} = -\mathbf{X}^T \mathbf{W} \mathbf{X}$$

with

$$W := diag(\hat{\mathbf{y}} \odot (\mathbf{1} - \hat{\mathbf{y}}))$$

Update rule for the Logistic Regression with Newton optimization:

$$\hat{\beta}^{(t)} := \hat{\beta}^{(t-1)} + \mu(\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T(\mathbf{y} - \hat{\mathbf{y}})$$

Learning Logistic Regression via Newton

learn-logreg-Newton$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \mu, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$\ell := -\log L_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) := \sum_{n=1}^{N} y_n \langle x_n, \hat{\beta} \rangle - \log(1 + e^{\langle x_n, \hat{\beta} \rangle})$

$\hat{\beta} :=$ minimize-Newton$(\ell, 0_M, \mu, t_{\max}, \epsilon)$

return $\hat{\beta}$

Newton Algorithm for the Loglikelihood

$x1$	$x2$	y
1	1	+
3	2	+
2	2	−
0	3	−

$$\mathbf{X} := \begin{pmatrix} 1 & 1 & 1 \\ 1 & 3 & 2 \\ 1 & 2 & 2 \\ 1 & 0 & 3 \end{pmatrix}, \mathbf{y} := \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \hat{\beta}^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \mu = 1$$

$$\hat{y}^{(0)} = \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}, \quad W^{(0)} = diag \begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{pmatrix}, \quad X^T (y - \hat{y}) = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

$$\left(X^T W^{(0)} X\right)^{-1} = \begin{pmatrix} 14.55 & -2.22 & -5.11 \\ -2.22 & 0.88 & 0.44 \\ -5.11 & 0.44 & 2.22 \end{pmatrix}, \quad \hat{\beta}^{(1)} = \begin{pmatrix} 2.88 \\ 0.44 \\ -1.77 \end{pmatrix}$$

Visualization Logistic Regression Models

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

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

and more detailed some **level curves**

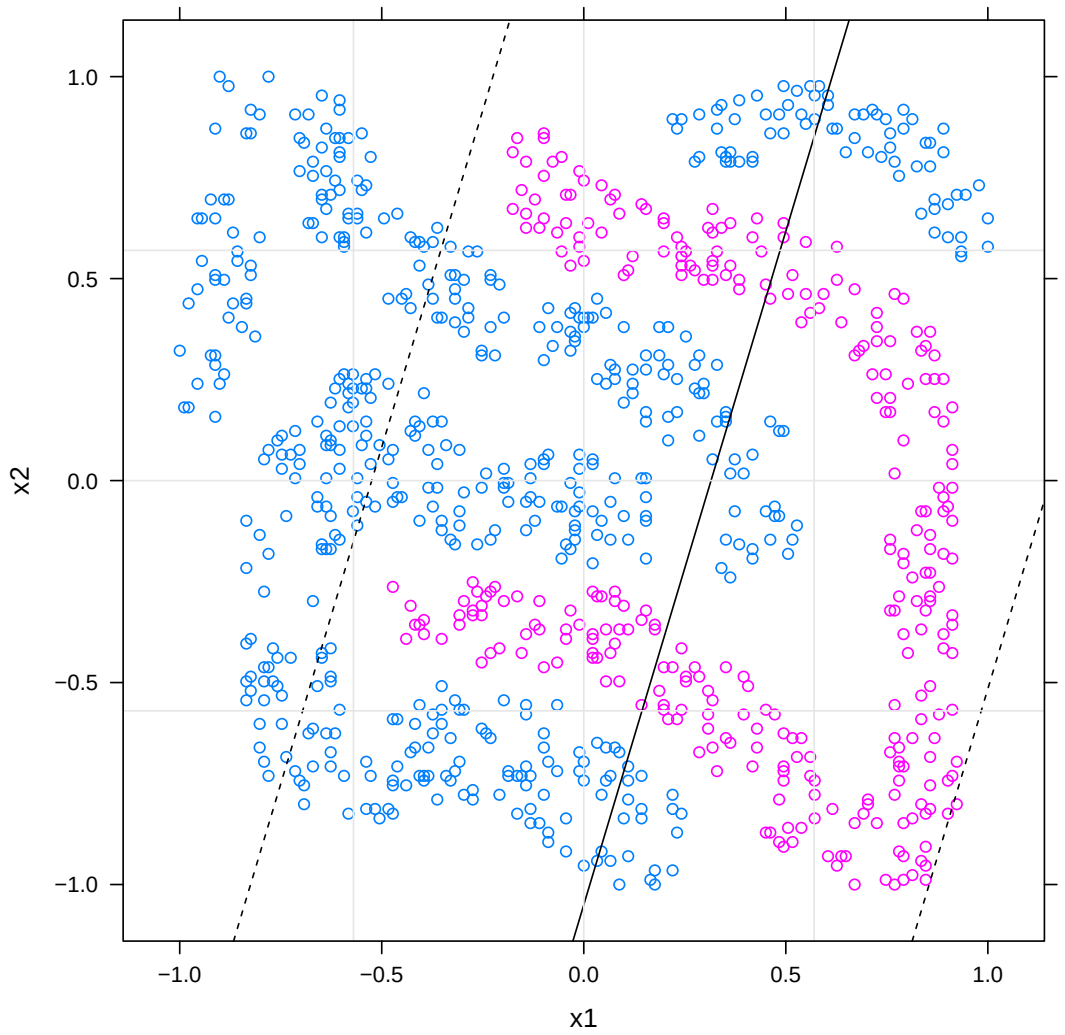
$$\hat{y}(X) = \hat{p}(Y = 1 \mid X) = p_0$$

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

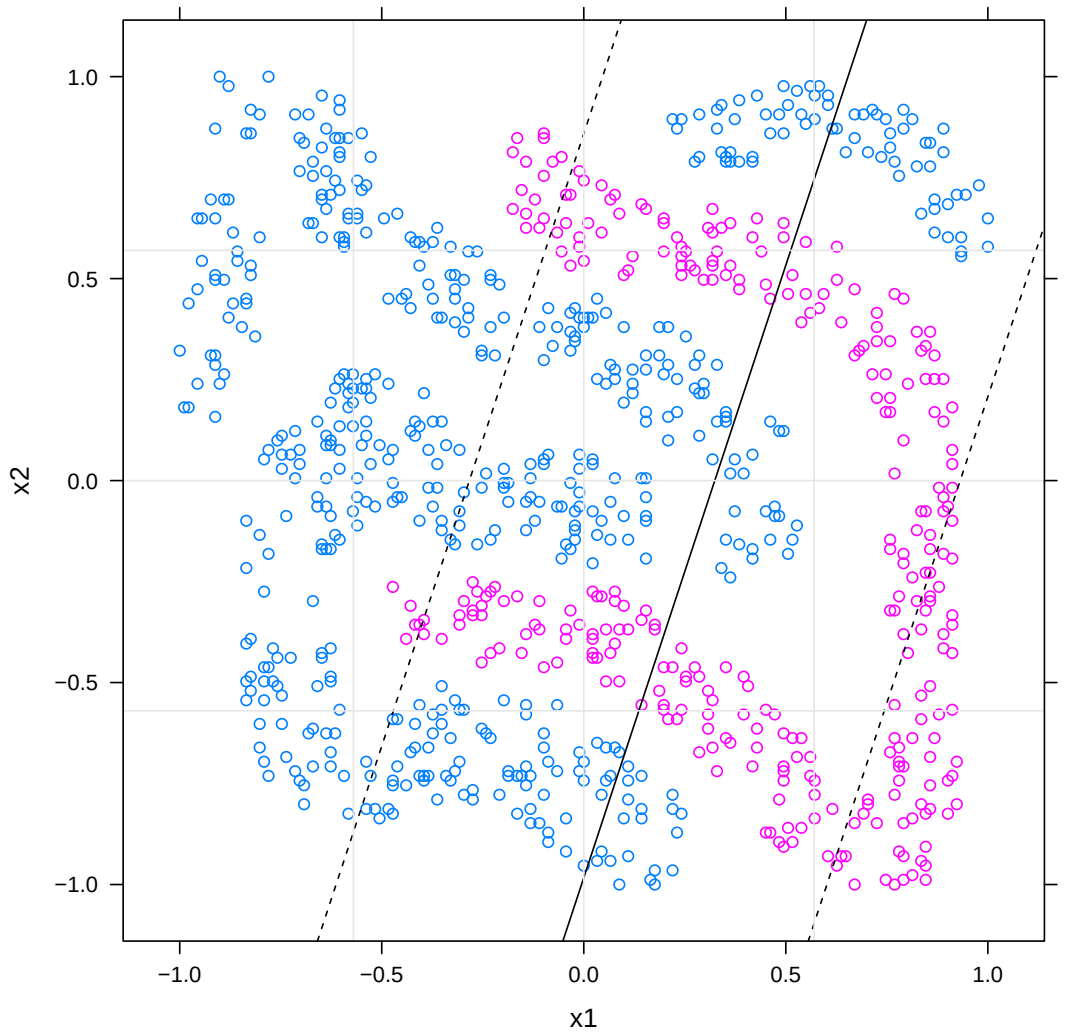
$$\langle \hat{\beta}, X \rangle = \log(\frac{p_0}{1 - p_0})$$

For logistic regression: decision boundary and level curves are straight lines!

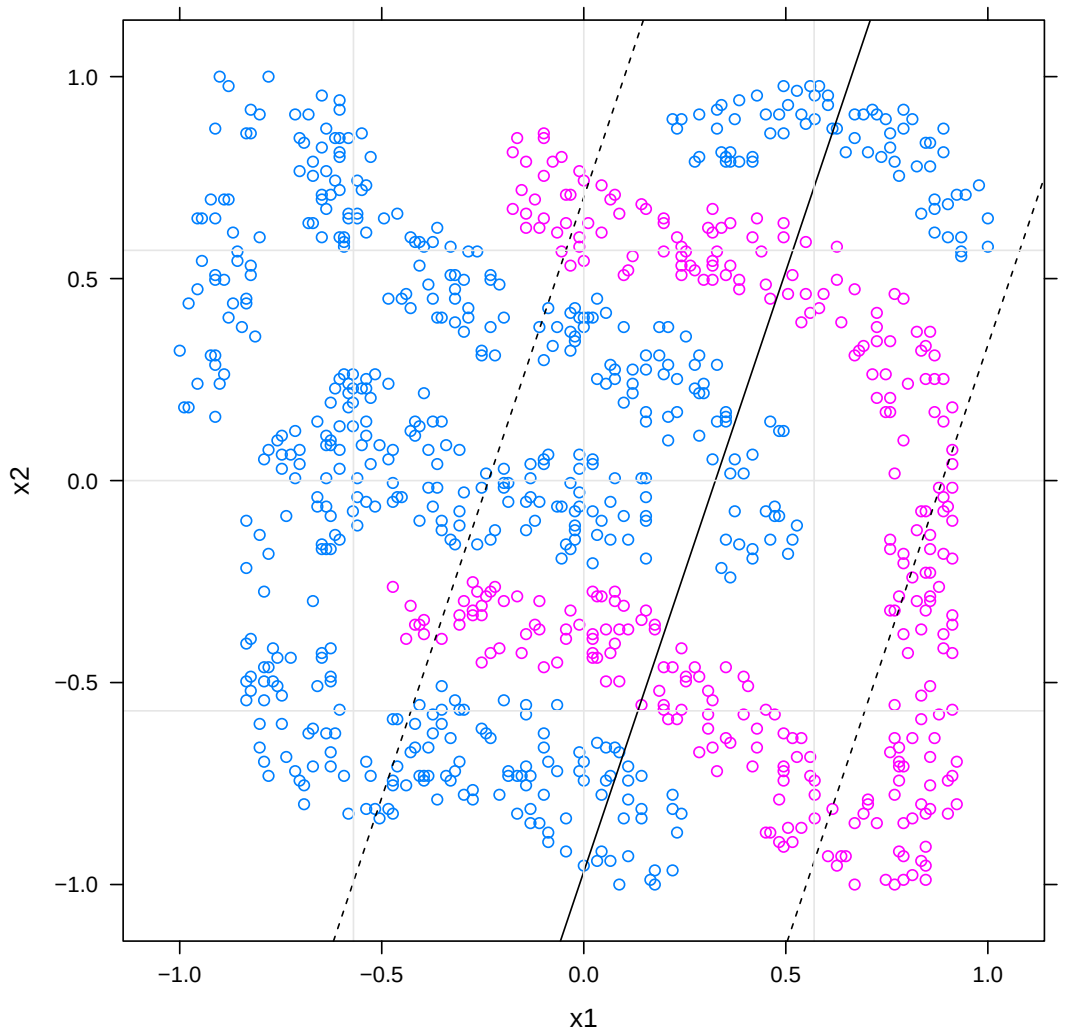
Visualization Logistic Regression Models ($t = 1$)



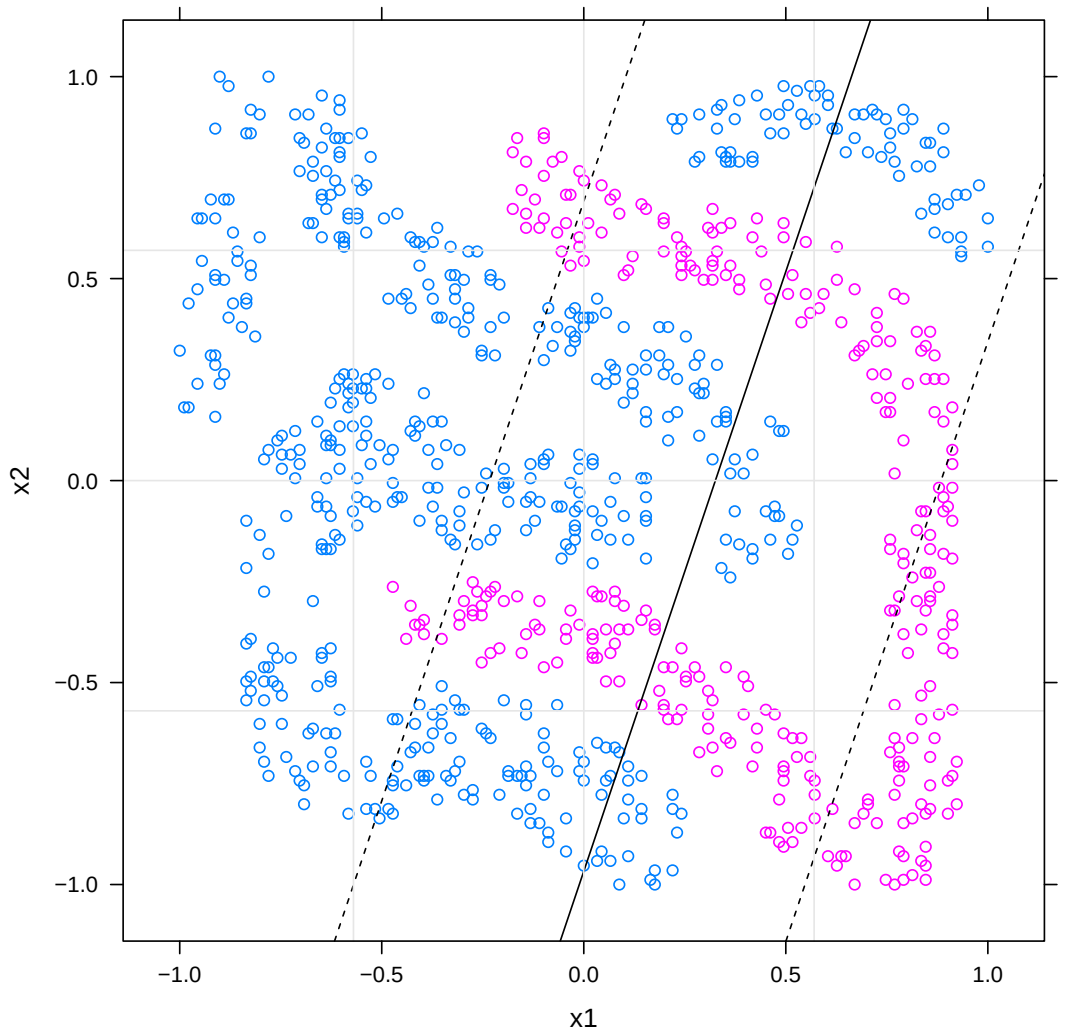
Visualization Logistic Regression Models ($t = 2$)



Visualization Logistic Regression Models ($t = 3$)



Visualization Logistic Regression Models ($t = 4$)



Outline

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.

Multi-class Targets as Multivariate Targets

- **multivariate regression**:

$$\hat{y}(x) = Bx + b, \quad B \in \mathbb{R}^{M \times T}, \quad b \in \mathbb{R}^{T}, \quad \hat{y}, \hat{y}(x) \in \mathbb{R}^{T}$$

  - can be learnt via gradient descent the same way as univariate regression
  - equivalent to T independent univariate regressions

- **Multi-class Logistic Regression**

$$\hat{y}(x) = \text{softmax}(Bx + b), \quad B \in \mathbb{R}^{M \times T}, \quad b \in \mathbb{R}^{T}, \hat{y}, \hat{y}(x) \in \mathbb{R}^{T}$$

$$\text{softmax}(z) := \left(\frac{e^{z_t}}{\sum_{t'=1}^{T} e^{z_{t'}}} \right)_{t=1:T}$$

  - can be learnt via gradient ascent the same way as univ. log. reg.
  - not equivalent to T independent logistic regressions, but different univariate targets learnt jointly.

Note: Multi-class Logistic Regression is also called **Multinomial Logistic**, **Maximum Entropy Classifier** or **Softmax Regression**.

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

Types of Compound Models

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

$$f_y : X \to [0,1], \quad y \in Y$$

$$f(x) := \left(\frac{f_1(x)}{\sum_{y \in Y} f_y(x)}, \ldots, \frac{f_k(x)}{\sum_{y \in Y} f_y(x)}\right)$$

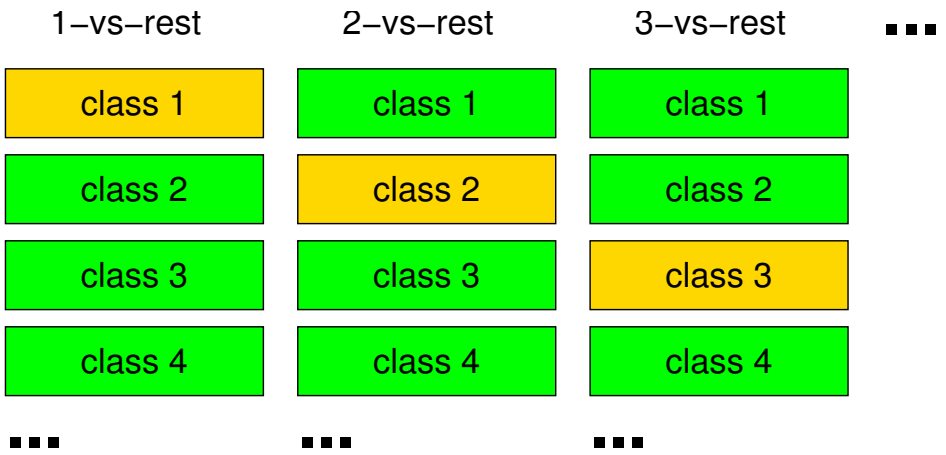
1-vs-last: one binary classifier per class (but last y_k):

$$f_y : X \to [0,1], \quad y \in Y, y \neq y_k$$

$$f(x) := \left(\frac{f_1(x)}{1 + \sum_{y \in Y} f_y(x)}, \ldots, \frac{f_{k-1}(x)}{1 + \sum_{y \in Y} f_y(x)}, \frac{1}{1 + \sum_{y \in Y} f_y(x)}\right)$$

Polychotomous Discrimination, k target categories

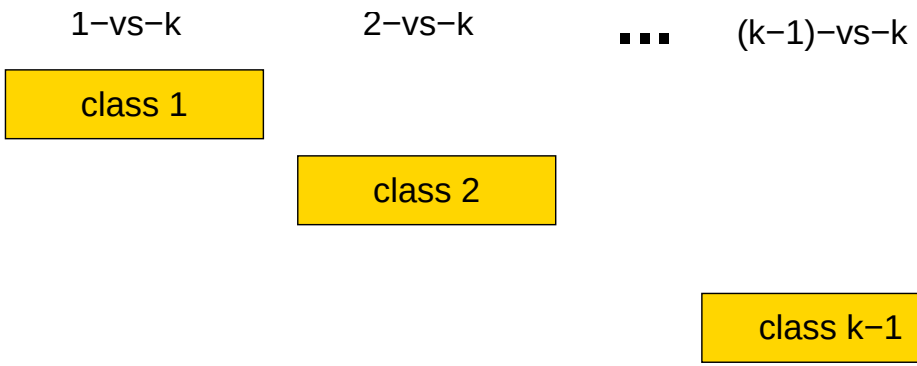
1-vs-rest construction:



k classifiers trained on N cases

kN cases in total

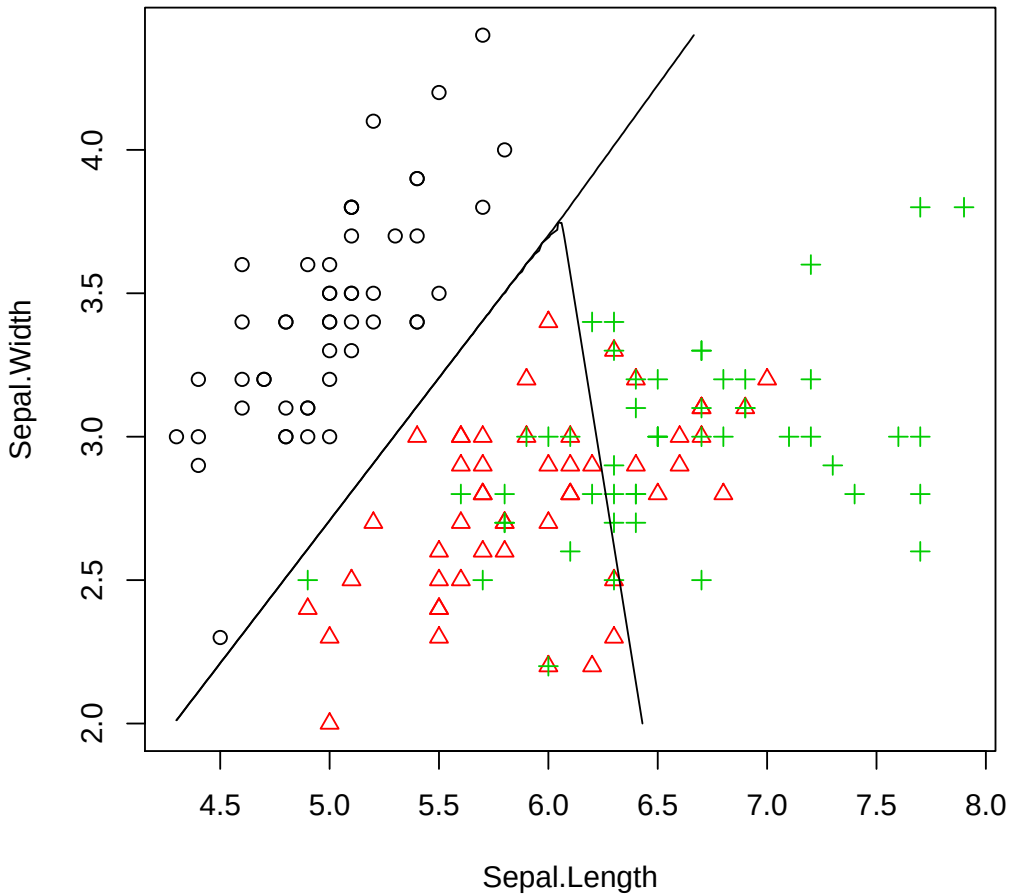
1-vs-last construction:



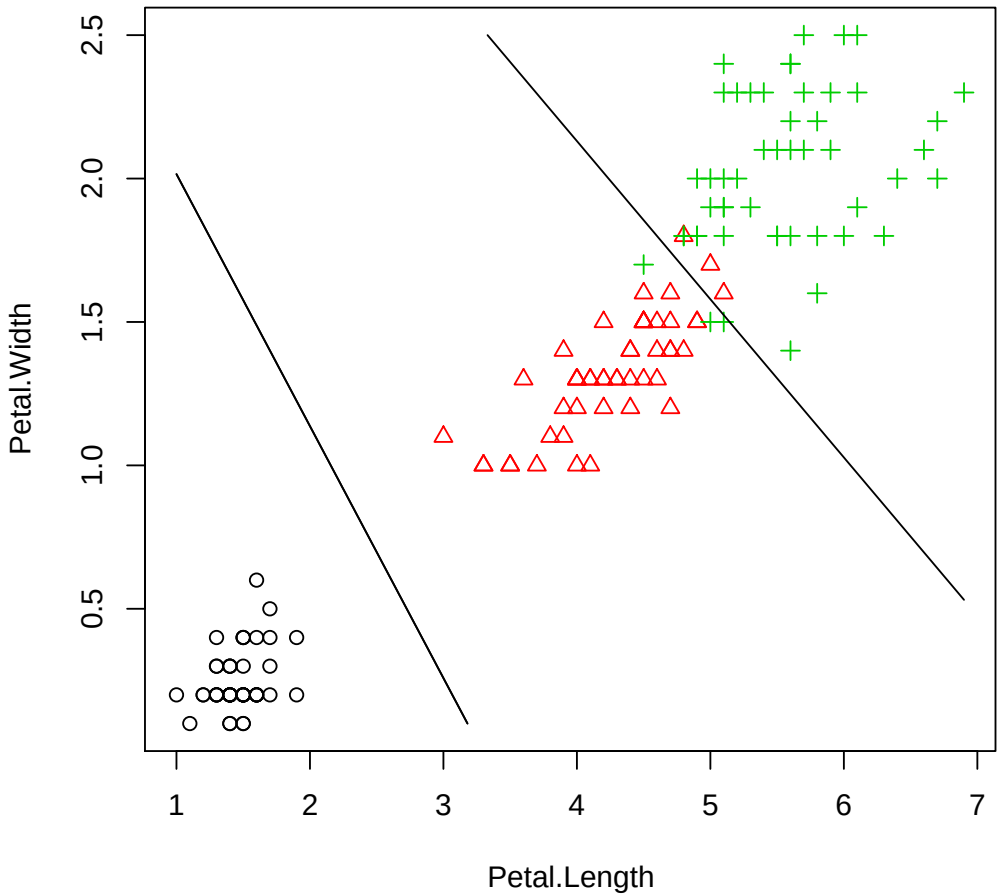
$k-1$ classifiers trained on approx. 2 N/k on average.

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

Example / Iris data / Logistic Regression



Example / Iris data / Logistic Regression



Outline

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

$$X \mid Y = k \sim \mathcal{N}(X \in \mathbb{R}^M \mid \mu_k, \Sigma_k)$$

i.e.

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

$$\mu_k \in \mathbb{R}^M, \Sigma_k \in \mathbb{R}^{M\times M}$$

Decision Rule

Discriminant analysis predicts as follows:

$$\hat{Y} \mid X = x := \arg\max_k \pi_k p_k(x) = \arg\max_k \delta_k(x)$$

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 **squared 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 to the class of the nearest prototype.

Maximum Likelihood Parameter Estimates

The maximum likelihood parameter estimates are as follows:

$$\hat{n}_k := \sum_{n=1}^{N} I(y_n = k), \quad \text{with } I(x = y) := \begin{cases} 1, & \text{if } x = y \\ 0, & \text{else} \end{cases}$$

$$\hat{\pi}_k := \frac{\hat{n}_k}{n}$$

$$\hat{\mu}_k := \frac{1}{\hat{n}_k} \sum_{n:y_n=k} x_n$$

$$\hat{\Sigma}_k := \frac{1}{\hat{n}_k} \sum_{n:y_n=k} (x_n - \hat{\mu}_k)(x_n - \hat{\mu}_k)^T$$

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.,

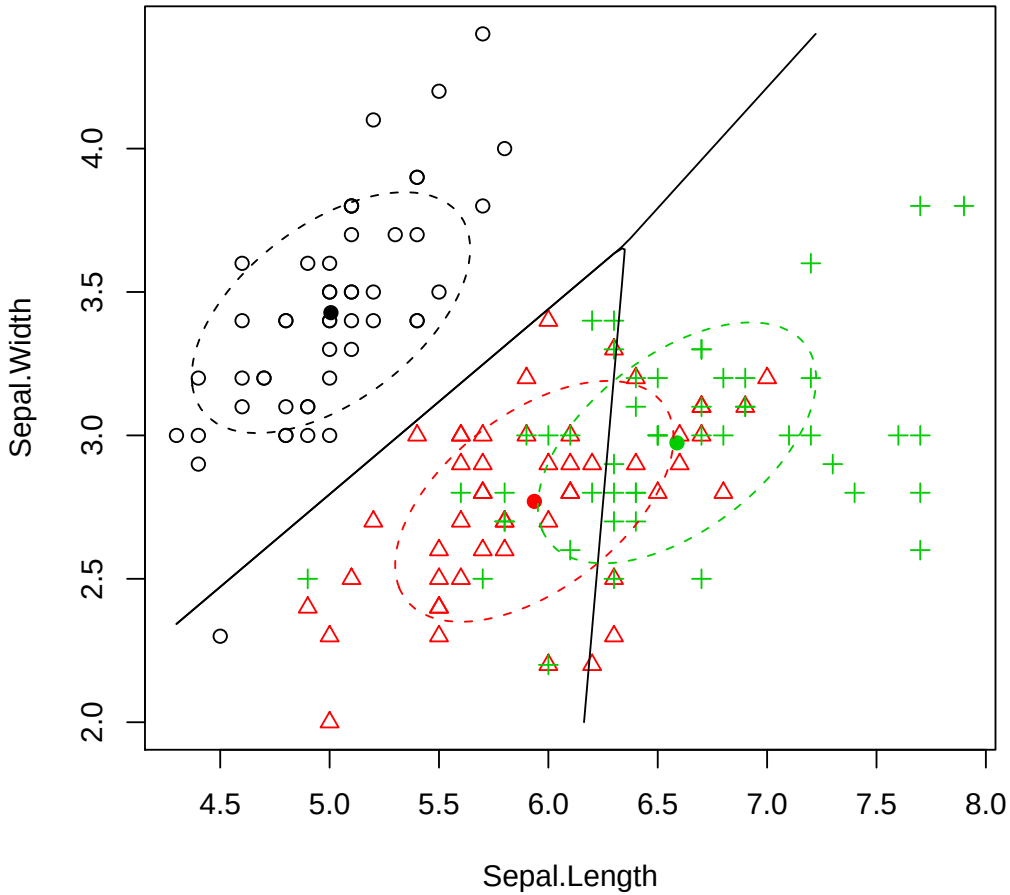
$$\Sigma_k = \Sigma_{k'} \quad \forall k, k'$$

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

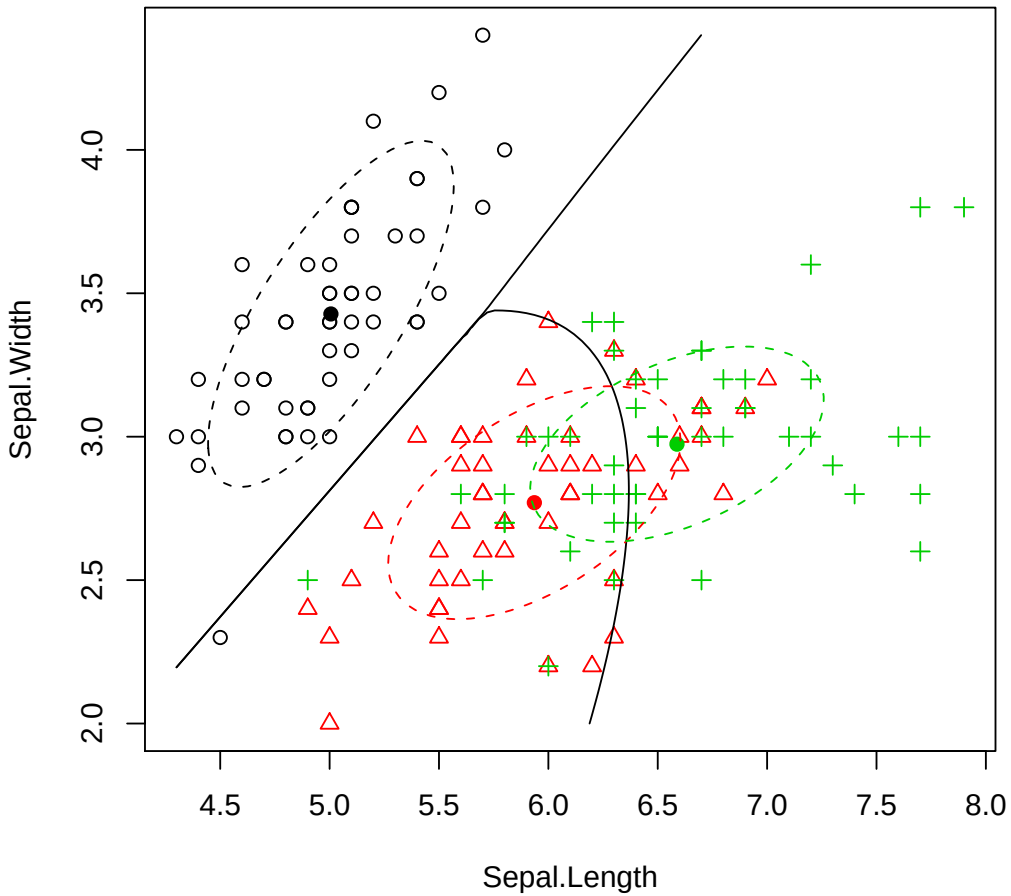
$$\hat{\Sigma} := \sum_k \frac{\hat{n}_k}{n} \hat{\Sigma}_k$$

Example / Iris data / LDA

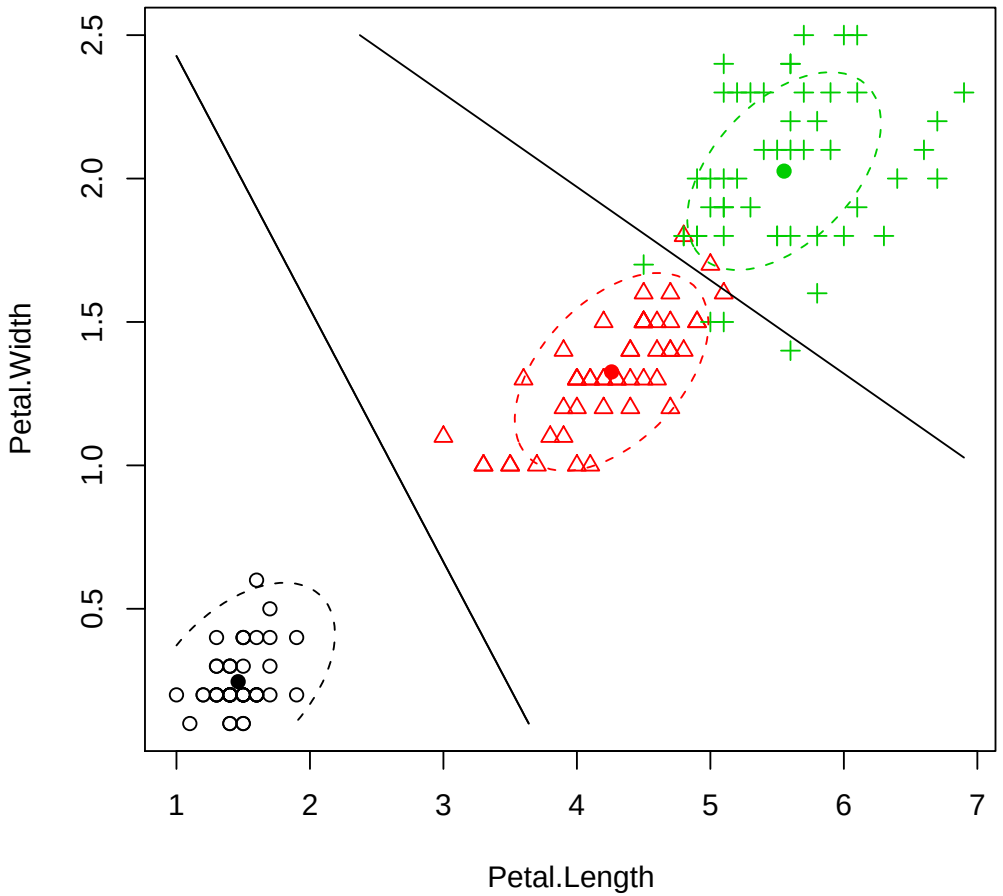


dashed curve: same distance to prototype
solid lines: same maximal probability for two classes

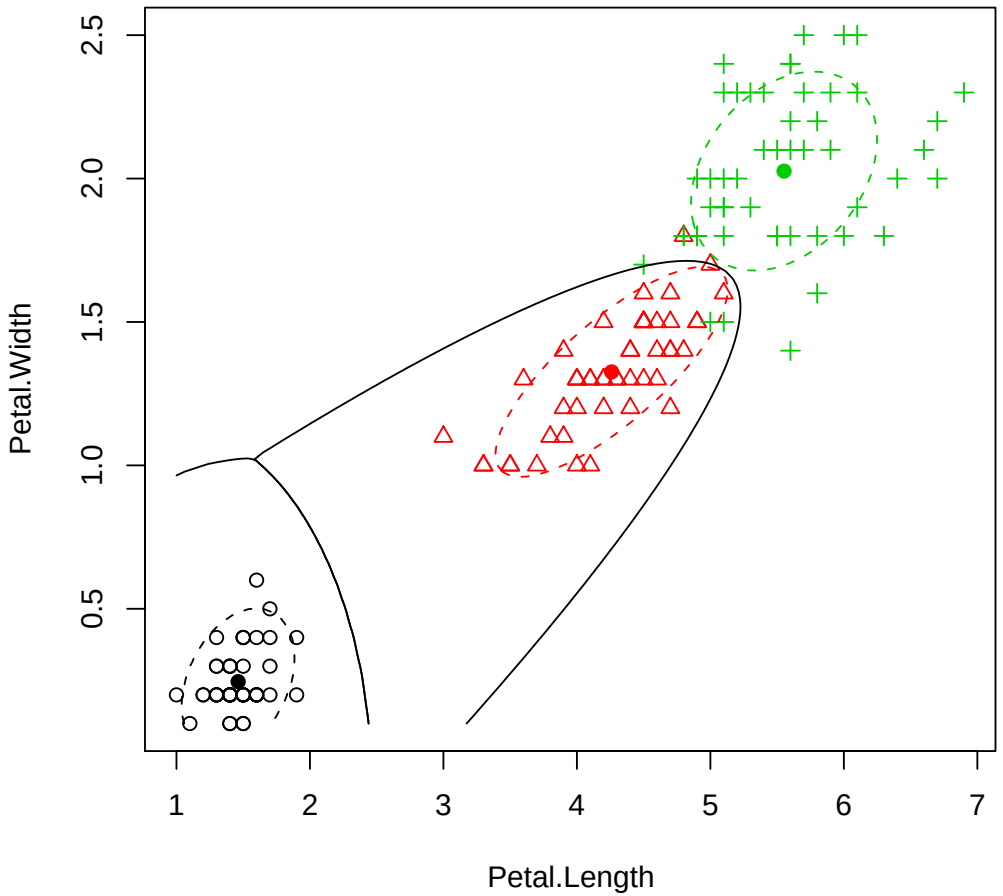
Example / Iris data / QDA



Example / Iris data / LDA



Example / Iris data / QDA



LDA coordinates

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

$$d(x, y) = \sqrt{\langle x - y, \hat{\Sigma}^{-1}(x - y)\rangle}$$

becomes the standard Euclidean distance in the transformed coordinates

$$d(x', y') = \sqrt{\langle x' - y', x' - y'\rangle} = \|x' - y'\|_2$$

This is accomplished by the **singular value decomposition** (SVD) of $\hat{\Sigma}$

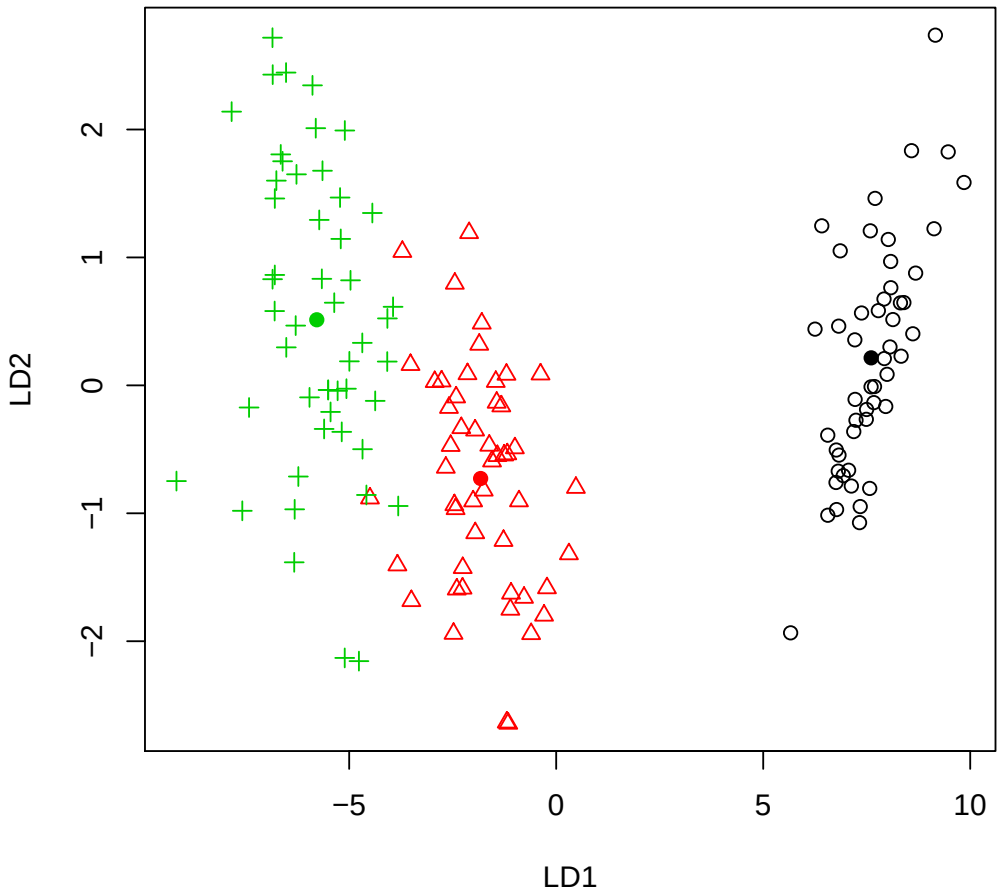
$$\hat{\Sigma} = UDU^T$$

with

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

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

Example / Iris data / LDA coordinates



LDA vs. Logistic Regression

LDA and logistic regression use the same underlying linear model.

For LDA:

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

For logistic regression by definition we have:

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

LDA vs. Logistic Regression

Both models differ in the way they estimate the parameters.

LDA maximizes the **complete likelihood**:

$$\prod_n p(x_n, y_n) = \underbrace{\prod_n p(x_n \mid y_n)}_{\text{normal } p_k} \quad \underbrace{\prod_n p(y_n)}_{\text{categorical } \pi_k}$$

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

$$\prod_n p(x_n, y_n) = \underbrace{\prod_n p(y_n \mid x_n)}_{\text{logistic}} \quad \underbrace{\prod_n f(x_n)}_{\text{ignored}}$$

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)** can be computed using
  - Gradient Ascent or
  - Newton's algorithm on the loglikelihood.
- 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**.

Further Readings

- [James et al., 2013, chapter 3], [Murphy, 2012, chapter 7], [Hastie et al., 2005, chapter 3].

References

Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin. *The Elements of Statistical Learning: Data Mining, Inference and Prediction*, volume 27. Springer, 2005.

Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani. *An Introduction to Statistical Learning*. Springer, 2013.

Kevin P. Murphy. *Machine Learning: A Probabilistic Perspective*. The MIT Press, 2012.