

Machine Learning

A. Supervised Learning A.2. Linear Classification

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Outline



- 1. The Classification Problem
- 2. Logistic Regression
 - 2.1. Logistic Regression with Gradient Ascent
 - 2.2. Logistic Regression with Newton
- 3. Multi-category Targets
- 4. Linear Discriminant Analysis

Outline



1. The Classification Problem

Logistic Regression 2.1. Logistic Regression with Gradient Ascent 2.2. Logistic Regression with Newton

- 3. Multi-category Targets
- 4. Linear Discriminant Analysis

Machine Learning 1. The Classification Problem

The Classification Problem

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

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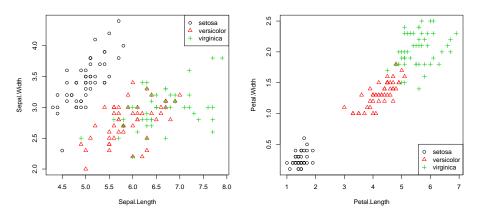
The Classification Problem

	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
÷	:	÷	÷	÷	
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

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The Classification Problem



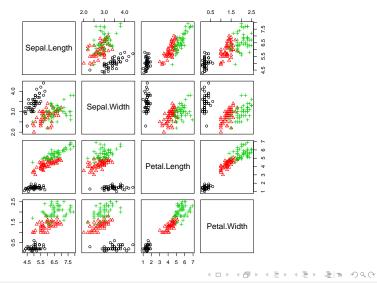
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The Classification Problem



Binary Classification



Lets start simple and consider two classes only. Lets say our target Y is $\mathcal{Y}:=\{0,1\}.$ Given

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

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**

$$\mathsf{err}(\hat{y};\mathcal{D}^{\mathsf{test}}) := rac{1}{|D^{\mathsf{test}}|} \sum_{(x,y)\in\mathcal{D}^{\mathsf{test}}} I(y
eq \hat{y}(x))$$

is minimal.

Note: $\mathcal{D}^{\text{test}}$ has (i) to be from the same data generating process and (ii) not to be available during training. $(\Box \mapsto (\Box) \to (\Box) \to (\Xi) \to (\Xi)$

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Binary Classification with Linear Regression

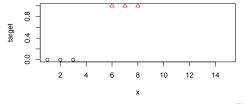
One idea could be to optimize the linear regression model

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

for RSS.

This has several problems

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



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Binary Classification with Linear Regression

Instead of predicting Y directly, we predict

 $p(Y = 1|X; \hat{\beta})$, the probability of Y being 1 knowing X.

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 $\left[0,1\right]$

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Logistic Function

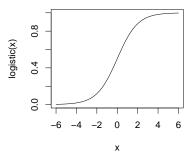
Logistic function:

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

The logistic function is a function that

- ▶ has values between 0 and 1,
- ► converges to 1 when approaching +∞,
- ► converges to 0 when approaching -∞,
- ► is smooth and symmetric at (0, 0.5).





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Maximum Likelihood Estimator Logistic regression model:

$$p(Y = 1 | X; \hat{\beta}) = \text{logistic}(\langle X, \hat{\beta} \rangle) + \epsilon = \frac{e^{\sum_{i=1}^{n} \hat{\beta}_{i} X_{i}}}{1 + e^{\sum_{i=1}^{n} \hat{\beta}_{i} X_{i}}} + \epsilon$$

As fit criterium, the likelihood is used.

As Y is binary, it has a Bernoulli distribution:

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

Thus, the conditional likelihood function is:

$$L_{D}^{\text{cond}}(\hat{\beta}) = \prod_{i=1}^{n} p(Y = y_i | X = x_i; \hat{\beta})$$

=
$$\prod_{i=1}^{n} p(Y = 1 | X = x_i; \hat{\beta})^{y_i} (1 - p(Y = 1 | X = x_i; \hat{\beta}))^{1-y_i}$$

Machine Learning 2. Logistic Regression

Estimating Model Parameters



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

This will be done by maximizing the conditional likelihood function $L_{\mathcal{D}}^{\text{cond}}$ which is in this case equivalent to maximizing the log likelihood $log(L_{\mathcal{D}}^{\text{cond}})$.

This can be done with any optimization technique, we will have a closer look at

- Gradient Ascent
- Newton

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Gradient Ascent

1: procedure

 $\begin{array}{ll} \text{MAXIMIZE-GA}(f:\mathbb{R}^{N} \to \mathbb{R}, \beta^{0} \in \mathbb{R}^{N}, \alpha, t_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^{+})\\ 2: \quad \text{for } t = 1, \dots, t_{\max} \text{ do}\\ 3: \quad \beta^{(t)} := \beta^{(t-1)} + \alpha \cdot \frac{\partial f}{\partial \beta}(\beta^{(t-1)})\\ 4: \quad \text{if } f(\beta^{(t)}) - f(\beta^{(t-1)}) < \epsilon \text{ then}\\ 5: \quad \text{return } \beta^{(t)} \end{array}$

6: **error** "not converged in t_{max} iterations"

For maximizing function f instead of minimizing it, we need to follow the positive direction of the gradient.

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Gradient Ascent for the Loglikelihood

$$\begin{split} \log \mathcal{L}_{\mathcal{D}}^{\text{cond}}(\hat{\beta}) &= \sum_{i=1}^{n} y_i \log p_i + (1 - y_i) \log(1 - p_i) \\ &= \sum_{i=1}^{n} y_i \log(\frac{e^{\langle x_i, \hat{\beta} \rangle}}{1 + e^{\langle x_i, \hat{\beta} \rangle}}) + (1 - y_i) \log(1 - \frac{e^{\langle x_i, \hat{\beta} \rangle}}{1 + e^{\langle x_i, \hat{\beta} \rangle}}) \\ &= \sum_{i=1}^{n} y_i(\langle x_i, \hat{\beta} \rangle - \log(1 + e^{\langle x_i, \hat{\beta} \rangle})) + (1 - y_i) \log(\frac{1}{1 + e^{\langle x_i, \hat{\beta} \rangle}}) \\ &= \sum_{i=1}^{n} y_i(\langle x_i, \hat{\beta} \rangle - \log(1 + e^{\langle x_i, \hat{\beta} \rangle})) + (1 - y_i)(-\log(1 + e^{\langle x_i, \hat{\beta} \rangle})) \\ &= \sum_{i=1}^{n} y_i\langle x_i, \hat{\beta} \rangle - \log(1 + e^{\langle x_i, \hat{\beta} \rangle}) \end{split}$$



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Gradient Ascent for the Loglikelihood

$$\log L_{D}^{\text{cond}}(\hat{\beta}) = \sum_{i=1}^{n} y_i \langle x_i, \hat{\beta} \rangle - \log(1 + e^{\langle x_i, \hat{\beta} \rangle})$$

$$\frac{\partial \log L_{D}^{\text{cond}}(\hat{\beta})}{\partial \hat{\beta}} = \sum_{i=1}^{n} y_i x_i - \frac{1}{1 + e^{\langle x_i, \hat{\beta} \rangle}} e^{\langle x_i, \hat{\beta} \rangle} x_i$$

$$= \sum_{i=1}^{n} x_i (y_i - p(Y = 1 | X = x_i; \hat{\beta}))$$

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

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



Gradient Ascent for the Loglikelihood

1: procedure LOG-REGR-

$$GA(L_{\mathcal{D}}^{cond}: \mathbb{R}^{P+1} \to \mathbb{R}, \hat{\beta}^{(0)} \in \mathbb{R}^{P+1}, \alpha, t_{max} \in \mathbb{N}, \epsilon \in \mathbb{R}^{+}$$

2: for $t = 1, ..., t_{max}$ do
3: $\hat{\beta}^{(t)} := \hat{\beta}^{(t-1)} + \alpha \cdot X^{T}(y - p)$
4: if $L_{\mathcal{D}}^{cond}(\hat{\beta}^{(t-1)}) - L_{\mathcal{D}}^{cond}(\hat{\beta}^{(t)})) < \epsilon$ then
5: return $\hat{\beta}^{(t)}$

6: **error** "not converged in t_{max} iterations"

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Newton Algorithm



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

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

$$F_n(\beta) := f(\beta_n) + \langle \frac{\partial f}{\partial \beta}(\beta_n), \beta - \beta_n \rangle + \frac{1}{2} \langle \beta - \beta_n, \frac{\partial^2 f}{\partial \beta \partial \beta^T}(\beta_n)(\beta - \beta_n) \rangle$$

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

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

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Newton Algorithm



Computing the derivative of the Taylor approximation with respect to x yields:

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

which leads to the Newton update:

$$\beta_{n+1} = \beta_n - \left(\frac{\partial^2 f}{\partial \beta \partial \beta^T}(\beta_n)\right)^{-1} \frac{\partial f}{\partial \beta}(\beta_n)$$

This requires inversion of the Hessian Matrix.

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Newton Algorithm

1: procedure

MINIMIZE-NEWTON $(f : \mathbb{R}^N \to \mathbb{R}, \beta^{(0)} \in \mathbb{R}^N, \alpha, t_{\mathsf{max}} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$

2: **for**
$$t = 1, \dots, t_{\max}$$
 do

3:
$$\beta^{(t)} := \beta^{(t-1)} - \alpha H^{-1} \nabla_{\beta} f$$

4: **if**
$$f(\beta^{(t-1)}) - f(\beta^{(t)}) < \epsilon$$
 then
5: **return** $\beta^{(t)}$

6: **error** "not converged in
$$t_{max}$$
 iterations"

 $\begin{array}{l} \beta^{(0)} \mbox{ start value} \\ \alpha \mbox{ (fixed) step length / learning rate} \\ t_{max} \mbox{ maximal number of iterations} \\ \epsilon \mbox{ minimum stepwise improvement} \\ H \in \mathbb{R}^{N \times N} \mbox{ Hessian matrix, } H_{i,j} = \frac{\partial^2 f}{\partial \beta_i \partial \beta_j} \\ \nabla_\beta f \in \mathbb{R}^N \mbox{ } (\nabla_\beta f)_i = \frac{\partial}{\partial \beta_i} f \end{array}$

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Newton Algorithm for the Loglikelihood

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

with

$$W := diag(\langle p, 1-p \rangle)$$

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

Update rule for the Logistic Regression with Newton optimization:

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

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Newton Algorithm for the Loglikelihood

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

$$p^{(0)} = \begin{pmatrix} 0.5\\ 0.5\\ 0.5\\ 0.5 \end{pmatrix}, \quad W^{(0)} = diag \begin{pmatrix} 0.25\\ 0.25\\ 0.25\\ 0.25 \end{pmatrix}, \quad X^{T} (y-p) = \begin{pmatrix} 0\\ 1\\ -1 \end{pmatrix}$$
$$\left(X^{T} W^{(0)} X\right)^{-1} = \begin{pmatrix} 14.55 & -2.22 & -5.11\\ -2.22 & 0.88 & 0.44\\ -5.11 & 0.44 & 2.22 \end{pmatrix}, \quad \hat{\beta}^{(1)} = \begin{pmatrix} 2.88\\ 0.44\\ -1.77\\ -1.77 \end{pmatrix}$$



Visualization Logistic Regression Models

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

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

and more detailed some level lines

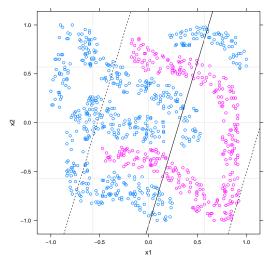
$$\hat{p}(Y=1\,|\,X)=p_0$$

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

$$\langle \hat{eta}, X
angle = \log(rac{p_0}{1-p_0})$$

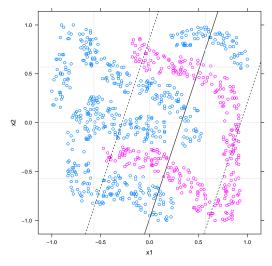


Decision Boundary after One Newton Step





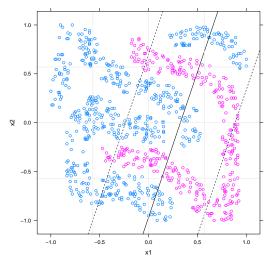
Decision Boundary after Two Newton Steps



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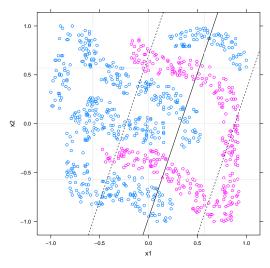
Decision Boundary after Three Newton Steps



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Decision Boundary after Four Newton Steps



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Machine Learning 3. Multi-category Targets

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.

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)
- 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:

$$\begin{aligned} f_y : X \to [0,1], \quad y \in Y \\ f(x) &:= \big(\frac{f_1(x)}{\sum_{y \in Y} f_y(x)}, \dots, \frac{f_k(x)}{\sum_{y \in Y} f_y(x)}\big) \end{aligned}$$

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

$$f_{y}: X \to [0,1], \quad y \in Y, y \neq y_{k}$$

$$f(x) := (\frac{f_{1}(x)}{1 + \sum_{y \in Y} f_{y}(x)}, \dots, \frac{f_{k-1}(x)}{1 + \sum_{y \in Y} f_{y}(x)}, \frac{1}{1 + \sum_{y \in Y} f_{y}(x)})$$

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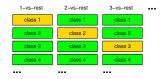


Machine Learning 3. Multi-category Targets

Polychotomous Discrimination, k target categories



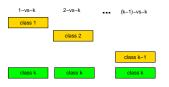
1-vs-rest construction:



k classifiers trained on N cases

kN cases in total

1-vs-last construction:



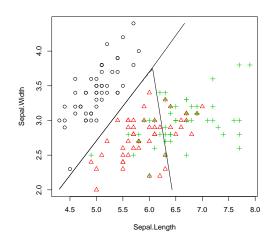
k-1 classifiers trained on approx. 2 N/k on average.

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

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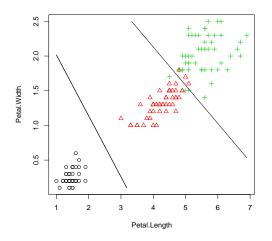
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Example / Iris data / Logistic Regression





Example / Iris data / Logistic Regression



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Assumptions

In discriminant analysis, it is assumed that

 \blacktriangleright cases of a each class k are generated according to some probabilities

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

and

i.e.

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

$$egin{aligned} X|Y &= k \sim \mathcal{N}(\mu_k, \Sigma_k) \ p_k(x) &:= rac{1}{(2\pi)^{rac{d}{2}}|\Sigma_k|^{rac{1}{2}}} e^{-rac{1}{2}\langle x-\mu_k, \Sigma_k^{-1}(x-\mu_k)
angle} \end{aligned}$$

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Decision Rule

Discriminant analysis predicts as follows:

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

with the discriminant functions

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

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 (with respect to Mahalanobis distance) prototype.

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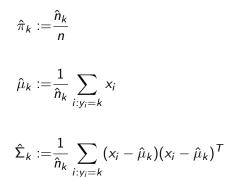




Maximum Likelihood Parameter Estimates

The maximum likelihood parameter estimates are as follows:

$$\hat{n}_k := \sum_{i=1}^n I(y_i = k), \quad \text{with } I(x = y) := \left\{ egin{array}{c} 1, & ext{if } x = y \\ 0, & ext{else} \end{array}
ight.$$



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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

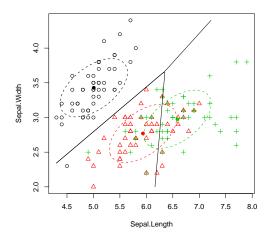
$$\hat{\Sigma} := \sum_{k} \frac{\hat{n}_{k}}{n} \hat{\Sigma}_{k}$$

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Example / Iris data / LDA

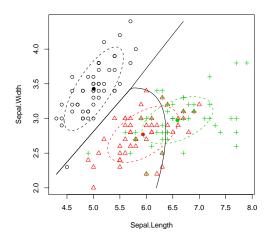




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Example / Iris data / QDA

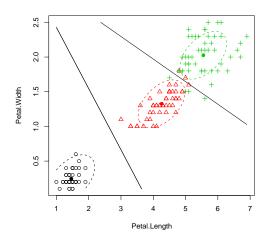




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Example / Iris data / LDA

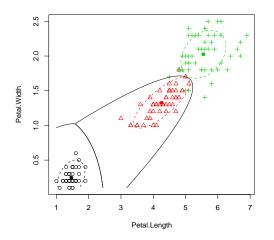




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Example / Iris data / QDA





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LDA coordinates

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

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

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

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

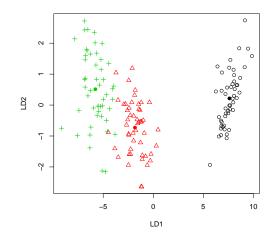
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Example / Iris data / LDA coordinates





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LDA vs. Logistic Regression



LDA and logistic regression use the same underlying linear model.

For LDA:

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

For logistic regression by definition we have:

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

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LDA vs. Logistic Regression

Both models differ in the way they estimate the parameters.

LDA maximizes the complete likelihood:

$$\prod_{i} p(x_{i}, y_{i}) = \prod_{i} p(x_{i} | y_{i}) \qquad \prod_{i} p(y_{i})$$

normal p_{k} bernoulli π_{k}

While logistic regression maximizes the conditional likelihood only:

$$\prod_{i} p(x_i, y_i) = \underbrace{\prod_{i} p(y_i \mid x_i)}_{\text{logistic}} \underbrace{\prod_{i} p(x_i)}_{\text{ignored}}$$

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Summary



- For classification, logistic regression models of type Y = ^{e⟨X,β⟩}/_{1+e⟨X,β⟩} + ε 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 π̂_k, μ̂_k, Σ̂ 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.

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Further Readings

► [JWHT13, chapter 3], [Mur12, chapter 7], [HTFF05, chapter 3].

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