

Lecture 2: Model-based classification

Rebecka Jörnsten, Mathematical Sciences

MSA220/MVE441 Statistical Learning for Big Data

24th March 2022



CHALMERS
UNIVERSITY OF TECHNOLOGY



UNIVERSITY OF GOTHENBURG

Recall: Statistical Learning (I)

Regression

- ▶ Theoretically best regression function for squared error loss

$$\hat{f}(\mathbf{x}) = \mathbb{E}_{p(y|\mathbf{x})}[y]$$

- ▶ Can be solved **data-driven** (1) or by **making model-assumptions** (2)
 1. k-nearest neighbour regression

$$\mathbb{E}_{p(y|\mathbf{x})}[y] \approx \frac{1}{k} \sum_{\mathbf{x}_{i_l} \in N_k(\mathbf{x})} y_{i_l}$$

2. linear regression (with implied constant β_0 and $x_0 = 1$)

$$\mathbb{E}_{p(y|\mathbf{x})}[y] \approx \mathbf{x}^T \boldsymbol{\beta}$$

Learning in Statistical Learning

Learn a model from data by minimizing expected prediction error determined by a loss function.

Expected prediction error

$$J(f) = \mathbb{E}_{p(\mathbf{x}, y)} [L(y, f(\mathbf{x}))] = \mathbb{E}_{p(\mathbf{x})} [\mathbb{E}_{p(y|\mathbf{x})} [L(y, f(\mathbf{x}))]]$$

How is this solved in practice, given a training sample $(y_l, \mathbf{x}_l)$ for $l = 1, \dots, n$?

1. Approximate $\mathbb{E}_{p(\mathbf{x}, y)} [L(y, f(\mathbf{x}))]$ from the training sample,

$$\text{i.e. } J(f) \approx \frac{1}{n} \sum_{l=1}^n L(y_l, f(\mathbf{x}_l)) \rightarrow \text{minimize w.r.t. } f$$

2. Find optimal theoretical solution (e.g. $\mathbb{E}_{p(y|\mathbf{x})}[y]$) and approximate it instead,

$$\text{e.g. } \mathbb{E}_{p(y|\mathbf{x})}[y] \approx \frac{1}{k} \sum_{\mathbf{x}_{i_l} \in N_k(\mathbf{x})} y_{i_l}$$

A third alternative

- ▶ Theoretically best regression function for squared error loss

$$\hat{f}(\mathbf{x}) = \mathbb{E}_{p(y|\mathbf{x})}[y]$$

if we allow **all functions!**

- ▶ Instead of approximating the overall optimal solution, we can restrict the class of allowed functions.
- ▶ **Example:** Restrict to class of **linear functions**, i.e.

$$f \in \{\mathbf{x} \mapsto \mathbf{x}^\top \boldsymbol{\beta} : \boldsymbol{\beta} \in \mathbb{R}^{p+1}\}$$

- ▶ Combined with squared error loss, the function minimizing (empirical) expected prediction error for the class of linear functions uses the standard least squares estimates $\hat{\boldsymbol{\beta}}$

Recall: Statistical Learning (II)

Classification

- ▶ Theoretically best classification rule for 0-1 loss and K possible classes

$$\hat{c}(\mathbf{x}) = \arg \max_{1 \leq i \leq K} p(i|\mathbf{x})$$

- ▶ Can be solved **data-driven** (1) or by **making model-assumptions** (2)
 1. k-nearest neighbour classification

$$p(i|\mathbf{x}) \approx \frac{1}{k} \sum_{\mathbf{x}_l \in N_k(\mathbf{x})} \mathbb{1}(i_l = i)$$

2. Instead of approximating $p(i|\mathbf{x})$ from data, can we make sensible model assumptions instead?

Model-based classification

A model for binary classification

Consider binary classification with $i = 0$ or $i = 1$.

We want to model $p(i|\mathbf{x})$ and since $p(0|\mathbf{x}) + p(1|\mathbf{x}) = 1$, it is enough to model one of the probabilities.

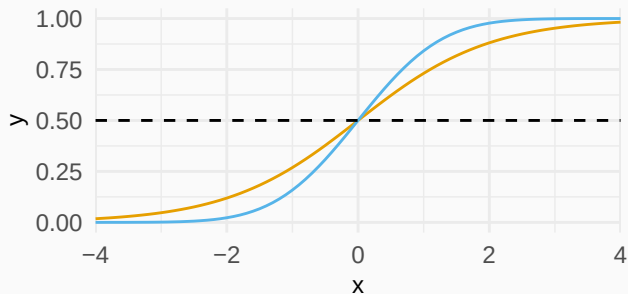
Bernoulli model:

- ▶ Let $p(1|\mathbf{x}) = \theta \in (0, 1)$, then $p(0|\mathbf{x}) = 1 - \theta$.
- ▶ Given responses i_l for $l = 1, \dots, n$ we can estimate the maximum likelihood estimate of θ
- ▶ Specifies a model approximation for **Bayes' rule**

$$c(\mathbf{x}) = \arg \max_{i \in \{0,1\}} p(i|\mathbf{x}) = \begin{cases} 0 & \theta \leq \frac{1}{2} \\ 1 & \text{otherwise} \end{cases}$$

How can we include predictors x_l ?

Logistic function and Normal Distribution CDF



Type — Logistic Function — Standard Normal CDF

Logistic (sigmoid) function

$$\sigma(x) = \frac{\exp(x)}{1 + \exp(x)}$$

Standard Normal CDF

$$\Phi(x) = \int_{-\infty}^x \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) dz$$

Logistic/probit models

Include a **linear predictor** after transformation, i.e.

logistic model

$$p(1|\mathbf{x}) \approx \sigma(\mathbf{x}^\top \boldsymbol{\beta})$$

probit model

$$p(1|\mathbf{x}) \approx \Phi(\mathbf{x}^\top \boldsymbol{\beta})$$

with corresponding Bayes' rule

$$c(\mathbf{x}) = \begin{cases} 0 & \mathbf{x}^\top \boldsymbol{\beta} \leq 0 \\ 1 & \text{otherwise} \end{cases}$$

since $\sigma(\mathbf{x}^\top \boldsymbol{\beta}) \leq 1/2$ for $\mathbf{x}^\top \boldsymbol{\beta} \leq 0$ and analogous for the probit model.

How are the regression coefficients determined?

The maximum likelihood estimates of β in the **logistic regression model** can be determined from the log-likelihood (with $i_l^* = 2i_l - 1$)

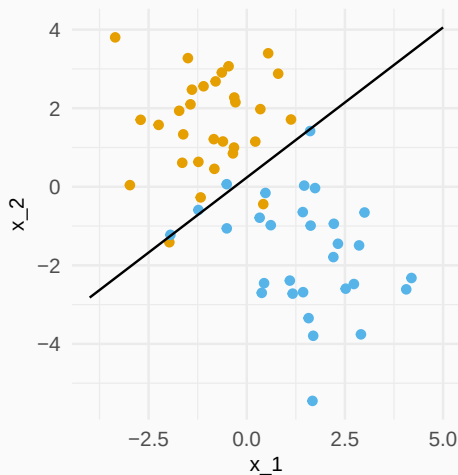
$$\begin{aligned} l(\beta) &= \sum_{l=1}^n i_l \log(\sigma(\mathbf{x}_l^\top \beta)) + (1 - i_l) \log(1 - \sigma(\mathbf{x}_l^\top \beta)) \\ &= \sum_{l=1}^n i_l^* \mathbf{x}_l^\top \beta - \log(1 + \exp(i_l^* \mathbf{x}_l^\top \beta)) \end{aligned}$$

The gradient is (with $\sigma(-x) = -\sigma(x)$)

$$\nabla_{\beta} l(\beta) = \sum_{l=1}^n i_l^* \mathbf{x}_l - \sigma(i_l^* \mathbf{x}_l^\top \beta) i_l^* \mathbf{x}_l = \sum_{l=1}^n \mathbf{x}_l (i_l^* - \sigma(\mathbf{x}_l^\top \beta))$$

which can be used in **gradient ascent** or leads to a **iteratively reweighted least squares** problem via the **Newton-Raphson algorithm**. (Details in ESL Ch. 4.4.1)

Example: Logistic regression



Decision boundary
(black line)

$$\beta_0 + \mathbf{x}^T \boldsymbol{\beta} = 0$$

$$\Leftrightarrow x_2 = (-\beta_0 - \beta_1 x_1) / \beta_2$$

How can logistic regression be extended to $K > 2$ classes?

Multi-class logistic regression (I)

- ▶ Assume there are $K > 2$ classes.
- ▶ **Requirement:** Probabilities need to be modelled, i.e. $p(i|\mathbf{x}) \in (0, 1)$ for each class and $\sum_i p(i|\mathbf{x}) = 1$, and dependence on predictors $\mathbf{x}_l$ should be included
- ▶ Use a categorical/multinomial model with

$$p(1|\mathbf{x}) = \theta_1, \dots, p(K-1|\mathbf{x}) = \theta_{K-1}, p(K|\mathbf{x}) = \theta_K$$

where $\theta_j \in (0, 1)$ and $\sum_j \theta_j = 1$.

- ▶ **Softmax function:** $\sigma : \mathbb{R}^K \mapsto [0, 1]^K$ for $j = 1, \dots, K-1$

$$[\sigma(\mathbf{z})]^{(j)} = \frac{e^{z_j}}{\sum_{r=1}^K e^{z_r}} = \frac{e^{z_j - z_K}}{1 + \sum_{r=1}^{K-1} e^{z_r - z_K}}, \quad [\sigma(\mathbf{z})]^{(K)} = \frac{1}{1 + \sum_{r=1}^{K-1} e^{z_r - z_K}},$$

Note that $K-1$ inputs are enough to determine the softmax function and $z_K = 0$ could be imposed without loss of generality.

Multi-class logistic regression (II)

- ▶ Use that only $K - 1$ parameters are necessary and model for $i = 1, \dots, K - 1$

$$p(i|\mathbf{x}) = \frac{e^{\mathbf{x}^\top \boldsymbol{\beta}_i}}{1 + \sum_{r=1}^{K-1} e^{\mathbf{x}^\top \boldsymbol{\beta}_r}}, \quad p(K|\mathbf{x}) = \frac{1}{1 + \sum_{r=1}^{K-1} e^{\mathbf{x}^\top \boldsymbol{\beta}_r}}$$

- ▶ This method has many names: multi-class logistic regression, softmax regression, multinomial logistic regression, maximum entropy classifier, ...
- ▶ Note that for any $i \in \{1, \dots, K - 1\}$

$$\log \frac{p(i|\mathbf{x})}{p(K|\mathbf{x})} = \mathbf{x}^\top \boldsymbol{\beta}_i$$

the **log-odds** of class i vs K . Class K is called the **reference class**.

Multi-class logistic regression (III)

Model for $i = 1, \dots, K - 1$

$$p(i|\mathbf{x}) = \frac{e^{\mathbf{x}^\top \boldsymbol{\beta}_i}}{1 + \sum_{r=1}^{K-1} e^{\mathbf{x}^\top \boldsymbol{\beta}_r}}, \quad p(K|\mathbf{x}) = \frac{1}{1 + \sum_{r=1}^{K-1} e^{\mathbf{x}^\top \boldsymbol{\beta}_r}}$$

► Bayes rule

$$c(\mathbf{x}) = \arg \max_{i=1, \dots, K} p(i|\mathbf{x}) = \begin{cases} K & \text{if } \mathbf{x}^\top \boldsymbol{\beta}_i < 0 \text{ for all } i = 1, \dots, K - 1 \\ \arg \max_i \mathbf{x}^\top \boldsymbol{\beta}_i & \text{otherwise} \end{cases}$$

► Decision boundaries are found through $\mathbf{x}^\top \boldsymbol{\beta}_i = \mathbf{x}^\top \boldsymbol{\beta}_j$ and $\mathbf{x}^\top \boldsymbol{\beta}_i = 0$ for all $i, j = 1, \dots, K - 1$.

Multi-class logistic regression models can be estimated with a **Newton-Raphson algorithm**, **coordinate descent**, **neural networks**, ... (see ESL Ch. 4.4.1 for some pointers)

The most over-used dataset in the world

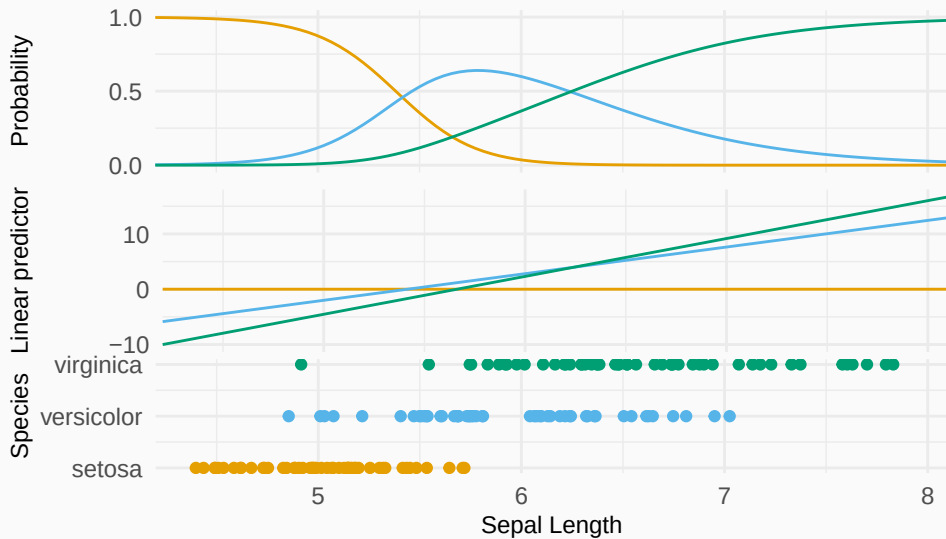
Iris flower data set

Measurements on iris flowers¹ collected by Edgar Anderson (published 1936)

- ▶ Three species: *iris setosa*, *iris virginica*, and *iris versicolor*
- ▶ 150 samples (50 for each species)
- ▶ Four features: Length and width of the sepals and petals in centimeters

¹https://en.wikipedia.org/wiki/Iris_flower_data_set#/media/File:Iris_versicolor_3.jpg

Multi-class logistic regression: An example



Notes on Logistic Regression

A warning: Problematic situation in two-class case (occurs seldom in practice)

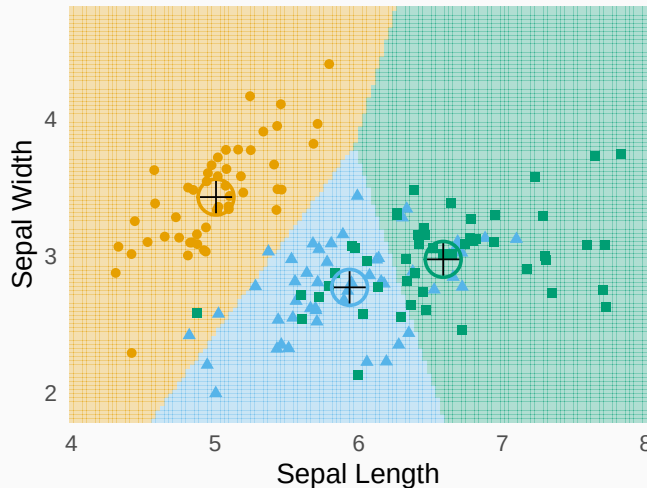
- ▶ Assume two classes can be separated perfectly by a line/hyperplane in predictor space. The classes are then called **linearly separable**.
- ▶ In this situation, logistic regression tries to fit a step-like function, which forces the intercept to $-\infty$ and the corresponding predictor coefficient to $+\infty$.
- ▶ Over-dispersion - more variance than model assumed - careful with p-values etc.

Big Data concerns:

- ▶ High-dimensional settings $\rightarrow$ non-identifiability of coefficients
- ▶ Interpretability in multiclass setting - different x s for different class models?
- ▶ Can use *regularization techniques* for these problems - more later.

Classification with focus on the feature/predictor space

Motivation for a different viewpoint: Nearest centroids



Species ● setosa ▲ versicolor ■ virginica

Determine mean predictor vector per class

$$\hat{\mu}_i = \frac{1}{n_i} \sum_{l=i} \mathbf{x}_l$$

where

$$n_i = \sum_{l=1}^n \mathbb{1}(i_l = i)$$

and classify points to the class whose mean is closest.

A change of scenery

So far

Classification problems can be solved by approximating $p(i|\mathbf{x})$ and applying Bayes' rule

- ▶ in a data-driven way, such as kNN,
- ▶ by a transformed regression model, as in logistic/probit regression

Observation: Good predictors group by class in feature space

Change of focus: Let's model the density of $\mathbf{x}$ conditionally on i instead!

How? **Bayes' law**

The setting of Discriminant Analysis

Apply Bayes' law

$$p(i|\mathbf{x}) = \frac{p(\mathbf{x}|i)p(i)}{\sum_{j=1}^K p(\mathbf{x}|j)p(j)}$$

Instead of specifying $p(i|\mathbf{x})$ we can specify

$$p(\mathbf{x}|i) \quad \text{and} \quad p(i)$$

The main assumption of Discriminant Analysis (DA) is

$$p(\mathbf{x}|i) \sim N(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$$

where $\boldsymbol{\mu}_i \in \mathbb{R}^p$ is the mean vector for class i and $\boldsymbol{\Sigma}_i \in \mathbb{R}^{p \times p}$ the corresponding covariance matrix.

Finding the parameters of DA

- ▶ Notation: Write $p(i) = \pi_i$ and consider them as unknown parameters
- ▶ Given data $(i_l, \mathbf{x}_l)$ the likelihood maximization problem is

$$\arg \max_{\mu, \Sigma, \pi} \prod_{l=1}^n N(\mathbf{x}_l | \mu_{i_l}, \Sigma_{i_l}) \pi_{i_l} \quad \text{subject to} \quad \sum_{i=1}^K \pi_i = 1.$$

- ▶ Can be solved using a Lagrange multiplier (try it!) and leads to

$$\hat{\pi}_i = \frac{n_i}{n}, \quad \text{with} \quad n_i = \sum_{l=1}^n \mathbb{1}(i_l = i)$$

$$\hat{\mu}_i = \frac{1}{n_i} \sum_{i_l=i} x_l$$

$$\hat{\Sigma}_i = \frac{1}{n_i - 1} \sum_{i_l=i} (x_l - \hat{\mu}_i)(x_l - \hat{\mu}_i)^\top$$

Performing classification in DA

Bayes' rule implies the classification rule

$$c(\mathbf{x}) = \arg \max_{1 \leq i \leq K} N(\mathbf{x} | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \pi_i$$

Note that since $\log$ is strictly increasing this is equivalent to

$$c(\mathbf{x}) = \arg \max_{1 \leq i \leq K} \delta_i(\mathbf{x})$$

where

$$\begin{aligned} \delta_i(\mathbf{x}) &= \log N(\mathbf{x} | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) + \log \pi_i \\ &= \log \pi_i - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^\top \boldsymbol{\Sigma}_i^{-1}(\mathbf{x} - \boldsymbol{\mu}_i) - \frac{1}{2} \log |\boldsymbol{\Sigma}_i| \quad (+ C) \end{aligned}$$

This is a quadratic function in $\mathbf{x}$.

Different levels of complexity

- ▶ This method is called **Quadratic Discriminant Analysis (QDA)**
- ▶ **Problem:** Many parameters that grow quickly with dimension
 - ▶ $K - 1$ for all π_i
 - ▶ $p \cdot K$ for all μ_i
 - ▶ $p(p + 1)/2 \cdot K$ for all Σ_i (most costly)
- ▶ **Solution:** Replace covariance matrices Σ_i by a pooled estimate

$$\hat{\Sigma} = \sum_{i=1}^K \hat{\Sigma}_i \frac{n_i - 1}{n - K} = \frac{1}{n - K} \sum_{i=1}^K \sum_{l_i=i} (x_l - \hat{\mu}_i)(x_l - \hat{\mu}_i)^{\top}$$

- ▶ **Simpler correlation and variance structure:** All classes are assumed to have the same correlation structure between features

Performing classification in the simplified case

As before, consider

$$c(\mathbf{x}) = \arg \max_{1 \leq i \leq K} \delta_i(\mathbf{x})$$

where

$$\delta_i(\mathbf{x}) = \log \pi_i + \mathbf{x}^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_i - \frac{1}{2} \boldsymbol{\mu}_i^\top \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_i \quad (+ C)$$

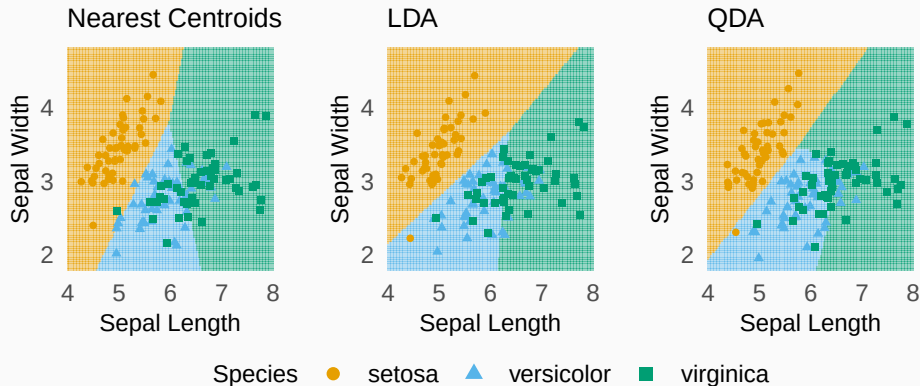
This is a linear function in $\mathbf{x}$. The method is therefore called **Linear Discriminant Analysis (LDA)**.

Even more simplifications

Other simplifications of the correlation structure are possible

- ▶ Ignore all correlations between features but allow different variances, i.e. $\Sigma_i = \Lambda_i$ for a diagonal matrix Λ_i (**Diagonal QDA** or **Naive Bayes' Classifier**)
- ▶ Ignore all correlations and make feature variances equal, i.e. $\Sigma_i = \Lambda$ for a diagonal matrix Λ (**Diagonal LDA**)
- ▶ Ignore correlations and variances, i.e. $\Sigma_i = \sigma^2 \mathbf{I}_{p \times p}$ (**Nearest Centroids adjusted for class frequencies π_i**)

Examples of LDA and QDA



Decision boundaries can be found with

$$N(\mathbf{x}|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)\pi_i = N(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)\pi_j \quad \text{for } i \neq j$$

and $\boldsymbol{\Sigma}_i = \boldsymbol{\Sigma}$ for LDA and $\boldsymbol{\Sigma}_i = \sigma^2 \mathbf{I}_{p \times p}$ for Nearest Centroids.

Summary and Big Data concerns

- ▶ Parametric classification - logistic regression.
 - ▶ Old friend - regression
 - ▶ Lots of tools, feature selection techniques, extensions to richer models
 - ▶ Penalized estimation for high-dimensional settings
 - ▶ Aggregation of estimates for large-sample settings
- ▶ Modelling the conditional densities of features instead of classes leads to Discriminant Analysis (DA)
 - ▶ There is a range of assumptions in DA about the correlation structure in feature space → trade-off between numerical stability and flexibility
 - ▶ High-dimensional case: simplify, simplify, ...
 - ▶ or... regularize: diagonal inflation - RDA. Lots of methods e.g. block-diagonal etc.
 - ▶ Flexible: don't need just one Gaussian shape for each class, can use a mixture of Gaussian shapes - FDA.