Machine Learning and Programming in Python

Lecture for Master and PhD students

Chair of Data Science in Economics

Ruhr University Bochum

Summer semester 2024

Lecture 6

Cross-validation

- Cross-validation is a resampling method
- Draw samples from the training data set, fit model, investigate how results differ for different samples
- For the methods of regularisation:
  choose λ via cross-validation

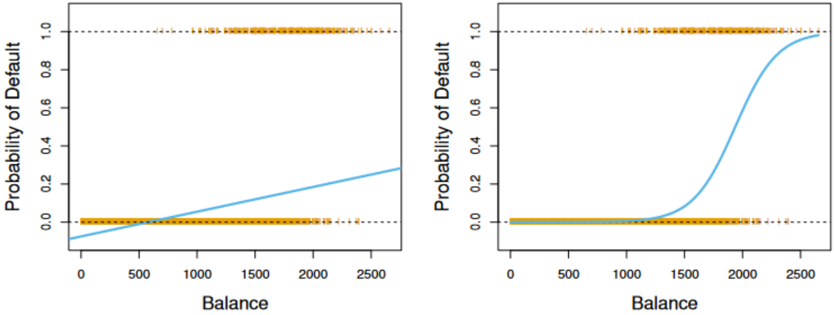
- k-fold cross-validation:
  - Randomly split the training data into k groups (folds) of roughly equal size
  - Pick a grid of λ values, and for each successive value:
    - Set aside the first fold as a validation set
    - Fit the model on the remaining folds, i=2,..,k
    - Compute the MSE_1 on the validation set
    - Repeat by using the second fold as the validation set and fitting on folds i=1,3,..,k
    - Compute the cross-validation error, $CV_k = \frac{1}{k}\sum_{i=1}^{k} MSE_i$
  - Select the λ which gives the lowest cross-validation error

Classification

- Classification methods are also an approach to **Supervised Learning**.
- Difference to regression problems: consider here a qualitative variable (instead of a quantiative variable for regression problems)

- Qualitative variables take values in an unordered set C, such as:
  eye color: *brown*, *blue*, *green*
  email: *spam*, *nospam*
- Given a feature vector X and a qualitative response Y taking values in the set C, the classification task is to build a function C(X) that takes as input the feature vector X and predicts its value for Y
- Often we are more interested in estimating the probabilities that X belongs to each category in C
- For example, it is more valuable to have an estimate of the probability that an insurance claim is fraudulent, than a classification fraudulent or not

- Suppose for the Default classification task that we code:
  Y = 0 if No and Y = 1 if Yes
- Can we simply perform a linear regression of Y on X and classify as Yes if $\hat{Y} > 0.5$?
  - In this case of a binary outcome, linear regression does a good job as a classifier
  - Since in the population $E(Y|X = x) = P(Y = 1|X = x)$, we might think that regression is perfect for this task.
  - However, linear regression might produce probabilities less than zero or bigger than one. Logistic regression is more appropriate.
- If we have a response variable with more than two possible values, and coding suggests an ordering, then linear regression is not appropriate $\Rightarrow$ Multiclass Logistic Regression or Discriminant Analysis are more appropriate



The orange data points indicate the response Y, either 0 or 1.
Linear regression does not estimate $P(Y = 1|X)$ well.
Logistic regression seems well suited to the task.

Logistic Regression

- Logistic regression uses the form:

  $$p(X) = P(Y = 1|X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

- $p(X)$ will have values between 0 and 1

- Log odds:

  $$log(\frac{p(X)}{1 - p(X)}) = \beta_0 + \beta_1 X$$

- We use maximum likelihood to estimate the parameters.
- $l(\beta_0, \beta) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0}(1 - p(x_i))$
- This likelihood gives the probability of the observed zeros and ones in the data. We pick β_0 and β_1 to maximize the likelihood of the observed data.
- We can compute the estimated probability $\hat{p}(X)$ at some X = x with the $\hat{\beta}$ coefficient estimates

- Having more than two classes: multi-class logistic regression = multinominal regression

$$\Pr(Y = k|X) = \frac{e^{\beta_{0k}+\beta_{1k}X_1+\ldots+\beta_{pk}X_p}}{\sum_{\ell=1}^{K} e^{\beta_{0\ell}+\beta_{1\ell}X_1+\ldots+\beta_{p\ell}X_p}}$$

Discriminant Analysis

- Here the approach is to model the distribution of X in each of the classes separately, and then use Bayes theorem to flip things around and obtain $P(Y|X)$.
- When we use normal (Gaussian) distributions for each class, this leads to linear or quadratic discriminant analysis.
- However, this approach is quite general, and other distributions can be used as well. We will focus on normal distributions

- Bayes theorem (for classification):

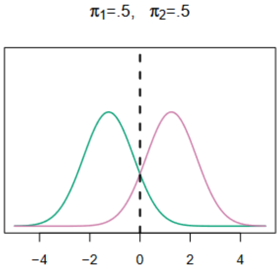
  $$P(Y = k|X = x) = \frac{P(X=x|Y=k)P(Y=k)}{P(X=x)}$$

- One writes this slightly differently for discriminant analysis:

  $P(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{k} \pi_l f_l(x)}$, where

  $f_k(x) = P(X = x|Y = k)$ is the density for X in class k. Here we will use normal densities for these, separately in each class

  $\pi_k = P(Y = k)$ is the marginal or prior probability for class k



- We classify a new point according to which density is highest.
- When the priors are different, we take them into account as well, and compare $\pi_k f_k(x)$. On the right, we favor the pink class - the decision boundary has shifted to the left

Why discriminant analysis?

- When the classes are well-separated, the parameter estimates for the logistic regression model are surprisingly unstable. Linear discriminant analysis does not suffer from this problem.
- If n is small and the distribution of the predictors X is approximately normal in each of the classes, the linear discriminant model is again more stable than the logistic regression model.
- Linear discriminant analysis is popular when we have more than two response classes, because it also provides low-dimensional views of the data

Linear Discriminant Analysis when p = 1

The Gaussian density has the form:

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma_k}\right)^2}$$

Here μ_k is the mean, and σ_k^2 k the variance (in class k). We will assume that all the $\sigma_k^2 = \sigma$ are the same.

Plugging this into Bayes formula, we get a rather complex expression:

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu_k}{\sigma}\right)^2}}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu_l}{\sigma}\right)^2}}$$

Discriminant functions

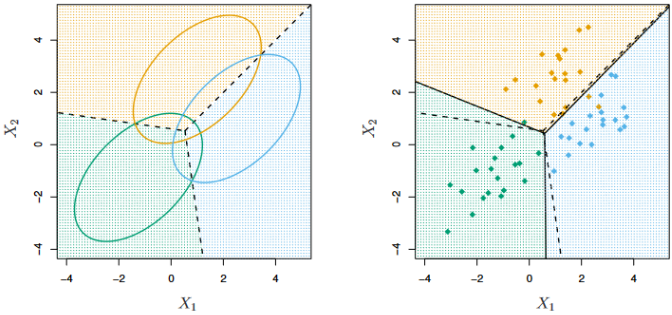
To classify at the value X = x, we need to see which of the $p_k(x)$ is largest. Taking logs, and discarding terms that do not depend on k, we see that this is equivalent to assigning x to the class with the largest discriminant score:

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

Note that $\delta_k(x)$ is a linear function of x.

If there are K = 2 classes and $\pi_1 = \pi_2 = 0.5$, then one can see that the decision boundary is at

$x = \frac{\mu_1 + \mu_2}{2}$.



Here p=2, K=3, $\pi_1 = \pi_2 = \pi_3 = 1/3$. The dashed lines are known as the Bayes decision boundaries. Were they known, they would yield the fewest misclassification errors, among all possible classifiers

- Once we have estimates $\hat{\delta}_k(x)$, we can turn these into estimates for class probabilities:

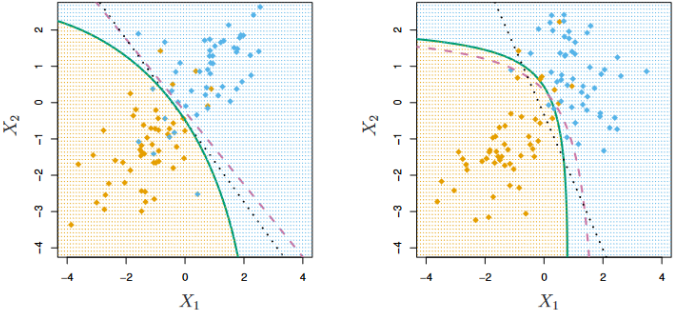
$$\hat{P}(Y = k|X = x) = \frac{e^{\hat{\delta}_k(x)}}{\sum_{l=1}^{K} e^{\hat{\delta}_l(x)}}$$

- So classifying to the largest $\hat{\delta}_k(x)$ amounts to classifying to the class for which $\hat{P}(Y = k|X = x)$ is largest.
- When K = 2, we classify to class 2 if $\hat{P}(Y = 2|X = x) >= 0.5$, else to class 1

Other forms of Discriminant Analysis

- $P(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$
- When $f_k(x)$ are Gaussian densities, with the same covariance matrix $\sum$ in each class, this leads to linear discriminant analysis. By altering the forms for $f_k(x)$, we get different classifiers.
  - With Gaussians but different $\sum_k$ in each class, we get quadratic discriminant analysis.
  - With $f_k(x) = \prod_{j=1}^{p} f_{jk}(x_j)$ (conditional independence model) in each class we get naive Bayes. For Gaussian this means the $\sum_k$ are diagonal.
  - Many other forms, by proposing specific density models for $f_k(x)$, including nonparametric approaches

Quadratic Discriminant Analysis



$$\delta_k(x) = -\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}_k^{-1}(x-\mu_k) + \log \pi_k - \frac{1}{2}\log|\Sigma_k|$$

Because the $\sum_k$ are different, the quadratic terms matter

Summary

- Logistic regression is very popular for classification, especially when K = 2.
- LDA is useful when n is small, or the classes are well separated, and Gaussian assumptions are reasonable. Also when $K > 2$.
- Many other classification methods available, e.g.
  - K-nearest neighbour (KNN): identify K points in training data, which lie closest to a point x_0, then assign x_0 to the class, which has the highest probability given the K points
  - Generalised Linear Models (GLM): Output variable is ordinal (count), methods: Poisson Regression, Gamma Regression, Negativ-Binomial Regression

Literature:

James, Witten, Hastie, Tibshirani, Taylor (2023), An Introduction to Statistical Learning, Springer, Chapter 4, pp. 135-161; Chapter 5, pp. 201-211.

Hastie, Tibshirani, Friedman (2017), The Elements of Statistical Learning, Springer, Chapter 4, pp. 106-111, pp. 119-122.