

Machine Learning Course - CS-433

Classification

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Minor changes by Nicolas Flammarion 2020, 2021; changes by Rüdiger Urbanke 2019, 2018, 2017, 2016; ©Mohammad Emtiyaz Khan 2015

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Classification

Similar to regression, [classification](#) relates the input variable \mathbf{x} to the output variable y , but now y can only take on discrete values. We say that y is a *categorical* variable.

Binary classification

When y can only take on two values, it is called [binary classification](#). Sometimes we refer to the two discrete values abstractly as $y \in \{\mathcal{C}_1, \mathcal{C}_2\}$. The \mathcal{C}_i are called [class labels](#) or simply [classes](#). Other times it is more convenient to assume that $y \in \{-1, +1\}$ or $y \in \{0, 1\}$. Note that even if the class labels are real values, there is typically no ordering implied between the two classes.

Multi-class classification

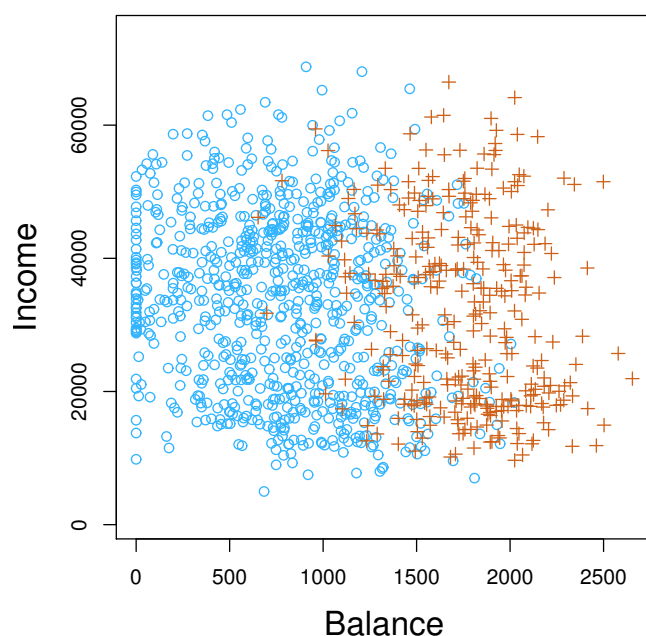
In a [multi-class classification](#), y can take on more than two values, i.e., $y \in \{\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_{K-1}\}$ for a K -class problem. Again, even though there is in general no ordering among these classes, we sometimes use the labels $y \in \{0, 1, 2, \dots, K-1\}$.

Examples of classification problems

A credit card service must be able to determine whether or not a requested transaction is fraudulent. They might have at their disposal the users IP address (if the transaction

happens on the web), past transaction history, and perhaps some other features.

An example from the book *Elements of Statistical Learning* by Hastie, Tibshirani, and Friedman is shown below. We have at our disposal the annual incomes and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card payments are shown in orange, and those who did not default are shown in blue.



To consider another example, a person arrives at the emergency room with a set of symptoms that could possibly be attributed to one of three medical conditions. Which of the three conditions does the individual have?

Classifier

A [classifier](#) will divide the input space into a collection of regions belonging to each class. The boundaries of these re-

gions are called **decision boundaries**. A classifier can be **linear** or **nonlinear**. This distinction is less strict than it might seem at first. E.g., if you look at the classifier in the right-hand side of “Figure 4.1” you will see that the decision regions are non-linear (not straight lines). But in fact the classifier that led to these region is linear – we added some non-linear features to the original feature vector (think polynomial basis) before performing the linear classification. The decision boundaries appear non-linear since the plot is made in the original feature space and not the extended feature space.

What is the aim of classification?

In some situations we are interested in classification in itself. This means, we are constructing a predictor based on a training set and are interested in applying this predictor to “new” data. Consider e.g. the example of the credit card company that wants to predict if a customer will default or not.

But in some instances we are interested in more. We would like to “understand” the cause. Think e.g. of a disease prediction. Not only are we interested to know who is at risk but we would like to understand *why* somebody is at risk. So we are interested in the “interpretation” of the prediction. In particular for this second task it is important to have *simple* models and to have means of eliminating features that do not contribute significantly to the prediction.

Consider “Figure 4.12”. In this data set various risk factors are given for a particular heart disease. These risk factors are blood pressure (sbp), tobacco usage, family history, obesity,

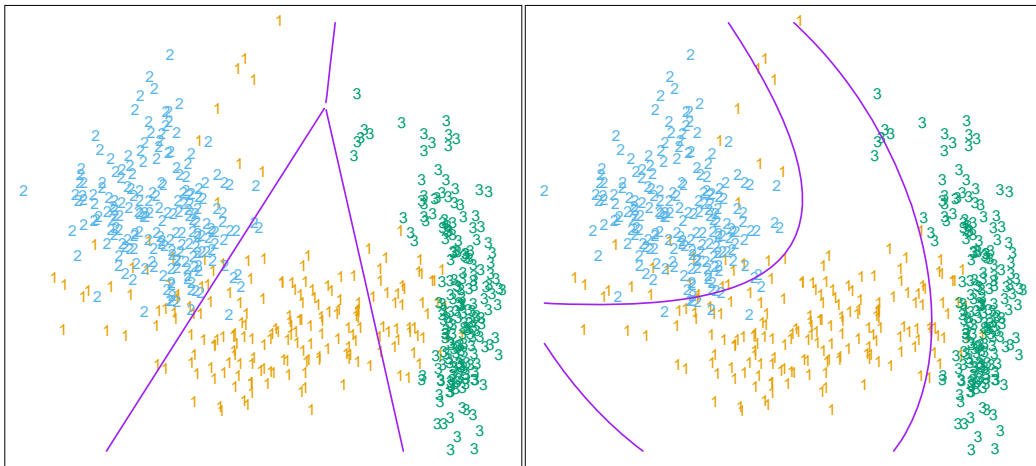


FIGURE 4.1. *The left plot shows some data from three classes, with linear decision boundaries found by linear discriminant analysis. The right plot shows quadratic decision boundaries. These were obtained by finding linear boundaries in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$. Linear inequalities in this space are quadratic inequalities in the original space.*

alcohol consumption, and age. For each pair of these risk factors the figure shows how the cases (people who have this disease) separate from the controls (people who do not have the disease). Such plots can help to decide which risk factors should be included in a model and which might have little predictive power.

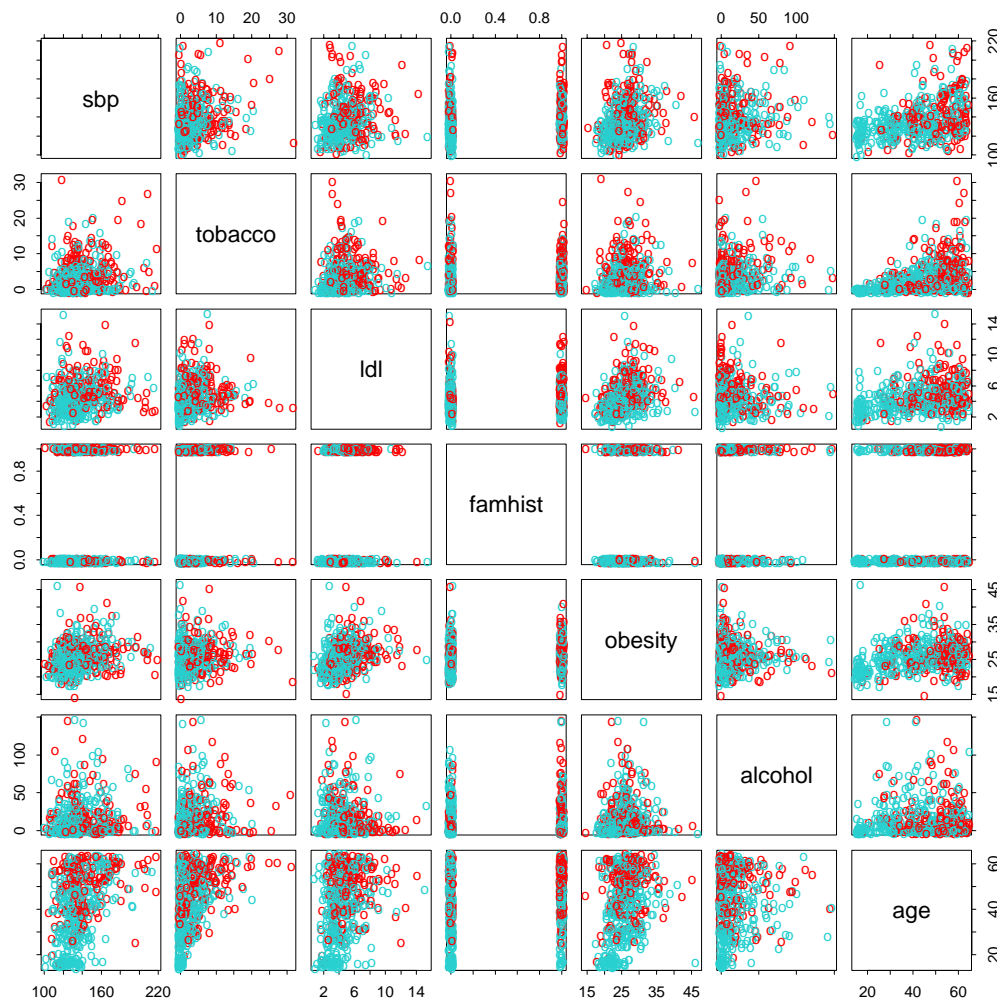


FIGURE 4.12. A scatterplot matrix of the South African heart disease data. Each plot shows a pair of risk factors, and the cases and controls are color coded (red is a case). The variable family history of heart disease (`famhist`) is binary (yes or no).

Classification as a special case of regression

From the very definition we see that classification is a *special case* of regression. It is a special case since the output is restricted to a small discrete set. So it might appear that there is not much new and that we should simply apply our

standard regression techniques to this special case.

E.g., we can assign $y = 0$ for \mathcal{C}_1 and $y = 1$ for \mathcal{C}_2 and, given a training set S_{train} , we can use (regularized) least-squares to learn a prediction function $f_{S_{\text{train}}}$ for this regression problem. To convert the regression into a classification it is then natural to decide on class \mathcal{C}_1 if $f_{S_{\text{train}}}(\mathbf{x}) < 0.5$ and \mathcal{C}_2 if $f_{S_{\text{train}}}(\mathbf{x}) > 0.5$.

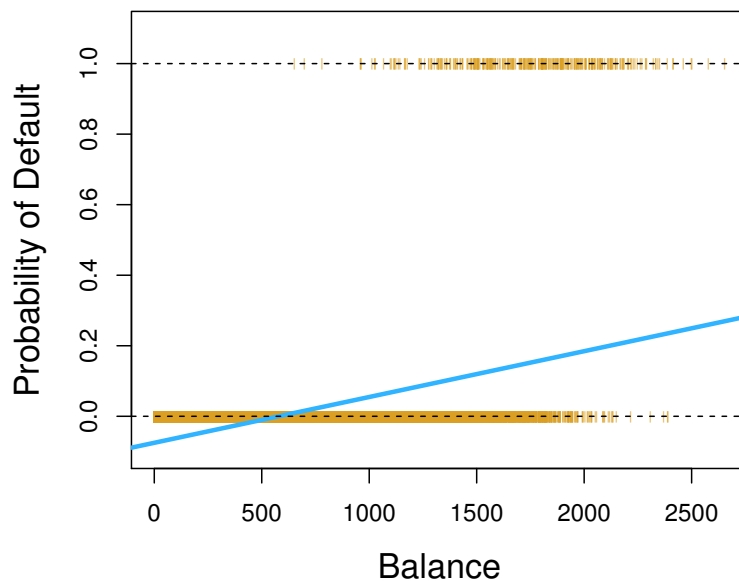
In the figure below this approach is applied to the credit-card default problem. To keep things simple we use as feature only the *balance* (as we have seen in a previous plot the second feature (the *income*) does not contain much information).

We think of $y = 0$ as “no default” and $y = 1$ as “default”. The dots we see correspond to the various data points and all dots are either on the line $y = 0$ or $y = 1$. The horizontal axis corresponds to the input \mathbf{x} , the *balance*.

In the figure the output y is labeled as *probability*. This is just a convenient way of interpretation. Since the desired label y is either 0 or 1 we can think of y as the probability of a default.

So let us now run a regression on the training data S_{train} . To keep things simple we run a linear regression and learn the linear function $f_{S_{\text{train}}}(\mathbf{x})$. The result is the blue curve that is indicated.

We might want to interpret the value $f_{S_{\text{train}}}(\mathbf{x})$ as the probability of a default and then assign a label depending on whether this “probability” is smaller or larger than 0.5. Of course, this “probability” can be negative or be larger than 1 so such an interpretation has to be taken with a grain of salt.



Why classification is not just a special case of regression

It is not hard to see that this method can lead to questionable results. Even if the cases and controls are well separated, the general “position” of the line will depend crucially on how many points are in each class and where these points lie. E.g., if we add a few points with $y = 1$ and a very large balance this will shift the curve significantly even though only a few points changed. This is clearly not a desirable property.

Why does this happen? The squared loss function that we used for regression is not a good match to our objective. We would like that the *fraction of misclassified cases* is small. But the mean-squared error is only very loosely related to this objective. In particular, the mean-squared error counts positive and negative deviations from the class label equally bad, although only one of them can potentially lead to a misclassification. If we do have a very small mean-squared error then indeed we can guarantee a small classification error

but the opposite is not true – a regression function can have arbitrarily large mean-squared error even though the fraction of misclassified cases is arbitrarily small. We therefore might have to work “much harder” than we should in bringing down the mean-squared error and so to have a guarantee on the misclassification error.

Based on the above observation, we see that classification is not just a special form of regression with a simple loss function like the mean-squared error.

Some basic ideas of how to perform classification

Many different approaches have been developed over the years of how to efficiently perform classification. Our aim right now is not to give an exhaustive account of all possible techniques. Rather, let us quickly discuss some basic ideas. We will come back and discuss those in more detail in later lectures.

Nearest Neighbor

In some cases it is reasonable to postulate that inputs that are “close” are also likely to have the same label attached. Here “close” might e.g. be measured by the Euclidean distance. If we believe that this assumption is good, then, given an input \mathbf{x} and a training set S_{train} , we can look for that point \mathbf{x}^* which is closest to \mathbf{x} and an element of S_{train} and then output y^* , the label attached to \mathbf{x}^* .

The good point about such a classifier is that it might work well even in cases where the decision boundaries are very irregular (see the Figure 2.3 below). But, as we will discuss in a later lecture, such a scheme fails miserably in high dimensions since in this case the geometry renders the notion of “close by” meaningless.

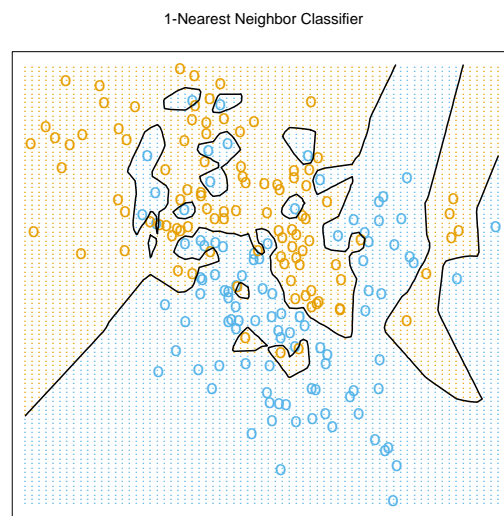


FIGURE 2.3. The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1), and then predicted by 1-nearest-neighbor classification.

There are many natural generalizations of this concept. Instead of using a single neighbor we can use let's say the k nearest neighbors or we can take a weighted linear combination of elements in our neighborhood. The latter idea leads to *smoothing kernels*.

Linear decision boundaries

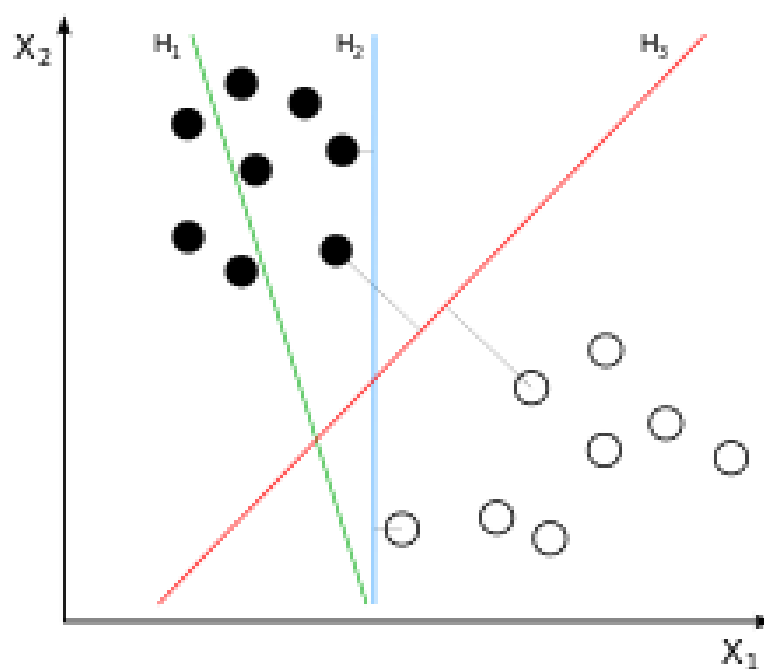
One starting point is to assume that decision boundaries are linear (hyperplanes). Consider e.g. a binary classification problem and look at schemes where the boundary between

the two classes is a hyperplane. We can ask how to pick this boundary. To keep things simple, assume that there exists a “separating hyperplane” i.e., a hyperplane so that no point in the training set is misclassified.

In general, there might be many hyperplanes that do the trick (assuming there is at least one). So which one should we pick?

One idea is to pick a hyperplane so that the decision has as much “robustness/margin” with respect to the training set as is possible. I.e., if we slightly change the training set by “wiggling” the inputs we would like that the number of misclassifications stays low.

In the figure below (taken from Wikipedia) we see that H_1 does not separate the data, but H_2 and H_3 do. Between H_2 and H_3 , H_3 is preferable, since it has a larger “margin.” This idea will lead us to [support vector machines](#) (SVM) as well as [logistic regression](#).



Non-linear decision boundaries

In many cases linear decision boundaries will not allow us to separate the data and non-linearities are needed. One option is to augment the feature vector with some non-linear functions. (The *kernel trick* is a method of doing this in an efficient way. We will learn about this at a later stage.)

Another way is to find an appropriate non-linear transform of the input so that the transformed input is then linearly separable. This is what is done when we are using *neural networks*.

Optimal classification for known generating model

It is instructive to think about how one could classify in an *optimal* fashion, i.e., how one could minimize the probability of misclassification, if the distribution of the generating model was known. To be concrete, assume that we know the joint distribution

$$p(\mathbf{x}, y)$$

and that y takes on elements in a discrete set \mathcal{Y} .

Given the “observation” (input \mathbf{x}), let $\hat{y}(\mathbf{x})$ be our estimate of the class label. What is the optimum choice for this function? Note that our estimate is only a function of the input \mathbf{x} . Further, for a given input \mathbf{x} , the probability that the “correct” label is y is $p(y \mid \mathbf{x})$, according to our model. So if our estimate is $\hat{y}(\mathbf{x})$ then we will be correct a fraction $p(\hat{y}(\mathbf{x}) \mid \mathbf{x})$ of the time. We conclude that if we want to maximize the probability of guessing the correct label then we should chose

the decision rule

$$\hat{y}(\mathbf{x}) = \operatorname{argmax}_{y \in \mathcal{Y}} p(y \mid \mathbf{x}).$$

This is called the [maximum a-posteriori](#) (MAP) criterion since we maximize the posterior probability (it is called posterior probability, since it is the probability of a class label *after* we have observed the input \mathbf{x}). This classifier is also called the Bayes classifier.

The probability of a correct guess is then the average (over all inputs \mathbf{x}) of this probability, i.e.,

$$\mathbb{P}\{\hat{y}(\mathbf{x}) = y\} = \int p(\mathbf{x})p(\hat{y}(\mathbf{x}) \mid \mathbf{x})dx.$$

In practice we do not know the joint distribution $p(\mathbf{x}, y)$. But we could use such an approach by using the data itself to learn the distribution (perhaps by assuming that the distribution is Gaussian and then just fitting the parameters from the data).