**Chapter 2: Overview of Statistical Learning**

2.1 Introduction to regression models

* The standard model for regression is , where is the ***reducible* error** (the error in prediction can be potentially reduced by choosing a different model) and is the ***irreducible error*** (it originates from e.g. measurement errors or inherent stochasticity and cannot be reduced by changing the model).
* A good will allow us to make predictions of the value of at new points of .
* The ideal function will give the expectation value of at :

This ideal function is called the ***regression function***. This ideal function is optimal is the optimal predictor of in the sense that it will minimize the ***sum of squared errors***.

* Typically, there will be very few, if any, data points that correspond to a certain value of (for example, there may be no values for the output data at exactly ). In that case the expectation value cannot be determined.
* In this case, is estimated based on the points in the ***neighbourhood*** of :

Where is some neighbourhood around . This is called ***Nearest Neighbour or Local averaging***.

2.2 Dimensionality and Structured Models

* Nearest neighbour averaging becomes more problematic as the number of dimensions increases: For a high number of dimensions, the width of the neighbourhood for nearest neighbour averaging needs to increase to capture the same number of data points.
* As a result, nearest neighbour averaging becomes less local for as the number of dimensions increases. This is called the ***Curse of Dimensionality***.
* The curse of dimensionality can be circumvented by using ***structural models*** that do not depend local properties and nearest neighbour averaging. An example of a structural model is a linear model for which each of the parameters can be found by fitting it to all datapoints. As a result, these linear models do not depend on any local properties or nearest neighbour averaging.
* Structural models that are less ***flexible*** (for example, linear vs. quadratic models) typically have lower ***interpretability***, although they may provide a better fit to the data.
* It is important to choose a model that is not too flexible to prevent ***overfitting*** of the data.

2.3 Model Selection and Bias-Variance Tradeoff

* To see how well a model performs, it can be fitted to a set of ***training data***:

However, this can be ***biased towards more overfit models***. Instead, the value should be evaluated on a set of ***test data***:

* The performance of models with different flexibilities can be assessed by plotting against model flexibility. The value of will typically have a minimum value for a certain flexibility of the model, while will keep decreasing as the model becomes more flexible.
* The choice for a certain flexibility of the model is subject to a ***Bias-Variance Tradeoff***: the variance in predictions of a model will increase as the model becomes more flexible (the model will become more sensitive to the peculiar characteristics of the training dataset). In return, the bias will decrease as the model becomes more flexible.

2.4 Classification

* In classification, the response variable is ***qualitative*** and the aim is to build a classifier that can assign a class label from the set of labels for future observations of .
* An ideal classifier is the ***Bayes Optimal Classifier*** that minimizes the probability of misclassification.
* If there are elements in the set of class labels then the ***Conditional Class Probabilities*** are:

The Bayes Optimal Classifier at is given by:

In other words, the Bayes Optimal Classifier assigns the observation to the ***most class with the highest probability***.

* In classification, nearest neighbour averaging can be used as in logistic regression (take the conditional probabilities in the neighbourhood of ). In that case, the curse of dimensionality still applies. However, the curse of dimensionality has less impact on than on .
* The performance of the classifier is typically measured using the ***Misclassification Rate***:

In words: ***the error is the average number of mistakes***. This error is the smallest for the Bayes Classifier.

* ***Support Vector Machines*** build structured models for **.**

**Chapter 3: Linear Regression**

3.1 Simple Linear Regression

* Linear regression is a simple approach to ***Supervised Learning*** (it is based on the assumption that the dependence of on is linear).
* Simplest case of linear regression is a model with a single predictor:

When the model coefficients have been estimated, the output can be predicted by:

* The best values for the parameters can be estimated by ***least squares***.
* The r***esidual*** (which is the discrepancy of the actual outcome with the predicted outcome) for the prediction of based on the value of is given by:

And the ***Residual Sum of Squares*** is:

* The unique line with values for and that minimizes the RSS is the ***least squares fit***.
* The accuracy of the estimates for and can be determined using the ***Standard Error***. The standard Error will ***increase when the variance () increases*** and the Standard Error will ***decrease when the spread of x-values around their mean increases***.
* The standard Errors can be used to define ***Confidence Intervals*** (For example, an interval that has a 95% probability to contain the true slope value).

3.2 Hypothesis testing and Confidence Intervals

* The standard error can also be used for performing ***Hypothesis Testing***. The most common Hypothesis test involves testing the Null Hypothesis:

***Null Hypothesis*** (): There is no relationship between and .

***Alternative Hypothesis*** (): There is some relationship between and .

* The Null Hypothesis is tested by computing a ***t-statistic:***

If the Null Hypothesis is true, this will ***have a t-distribution with degrees of freedom***.

* The ***p-value*** is the probability to get ***at least*** the obtained value for .
* ***Hypothesis Testing and using Confidence Tests are equivalent***: if one of the two shows that there is a relation between and then so will the other and vice versa. However, the Confidence Test also tells you how big the effect is.
* The accuracy of the model can be determined by computing the ***Residual Squared Error***:

And by computing the  ***value*** (the describes the fraction of the variance in the data that is explained by the model). , where is the correlation between and .

3.3 Multiple Linear Regression

* Multiple Linear Regression is regression with more than one predictor:
* How to interpret the different predictors now:

-***If the predictors are not correlated data***, each predictor can be interpreted separately.

-***Usually, the different predictors are correlated,***and this makes their interpretation much more complex. In addition, ***the variance on all coefficients can increase*** when the predictors are correlated. This is because the relation of a predictor to a certain variable is less strong in that case (the predictors of different variables can be swapped without significantly changing the result). In this case ***Claims od Causality*** should be avoided.

* The ***Least Squares Estimates*** can be determined in much the same way as for a simple linear model ().
* Instead of a line, the function will now be a ***Hyperplane***. Therefore, in this case the Least Squares Estimates minimize the distance between each data point and its closest point on this hyperplane.
* For multiple Linear Regression, the standard error, t-statistic and p-value will tell you whether one variable affects the outcome ***in the presence of the other variables***. Although a variable may not have a significant affect in the presence of other variables, it could have a significant effect on its own.
* ***The correlation between the variables*** will tell you something about whether the information on a certain variable significantly improves the prediction of the model given that you have information on the other variables. In other words, data on a variable may have become redundant in the presence of another variable when they are strongly correlated.

3.4 Some Important Questions

* Which of the predictors is useful for the prediction of the response? And how accurate is the prediction?
* To determine if any of the predictors is useful to predict the response, the ***-statistic*** is used:

Here, the  ***is the Total Sum of Squares***, which is the sum of the residuals when no model (the predictor of the data is the mean) is used. is the Residual Sum of Squares, which are the residuals that remain when using our predictive model. is the number of parameters in the model (in total parameters are fitted to the data, the accounts for the intercept) and is the sample size.

* In the case that there is no effect of the predictors (the null hypothesis), the ***-statistic will follow an -distribution with degrees of freedom ()*.**
* The values for the -distribution can be looked up in tables. ***A large -statistic indicates that there is a strong effect of the predictors on the response prediction.***
* To decide whether a variable is important for the prediction of a linear regression model, ***All subsets or best subsets regression*** can be used.
* In all subsets regression, the least squares fits for all possible subsets of variables are made and the best subset is chosen based on a balance between training error and model size.
* The problem with all subsets regression is that the number of models that need to be evaluated grows exponentially with the number of parameters in the model.
* Two commonly used approaches for all subsets regression:

***Forward Selection***

Starts with the ***null model*** (a model with only the intercept and no predictors). Then each of the variables is added one at a time to the null model and simple linear regressions are performed. ***The variable that results in the lowest is added to the null model***. This is repeated for two-variable models, three variable models etc., until some stopping rule is reached (such as ***all the remaining variables have a p-value above some threshold***).

***Backward Selection***

Start with a model that contains ***all the variables***. Then remove the variable that has the largest p-value (the one that is the least statistically significant) from the model. Repeat this process for a model with variables, variables etc., until some stopping rule is reached (such as ***all the remaining variables have a p-value below some threshold***).

* How to deal with ***Qualitative Variables*** instead of quantitative variables: incorporate a ***dummy variable*** in the model (there will always be one fewer dummy variable than the number of levels in the set of qualitative variables).

Such that the equation of the model becomes:

In this case ­will tell you the effect of belonging to class A versus the ***baseline***, which in this case corresponds to belonging to class B. The value of the intercept () represents the average value for for class B. The value of will represent the strength of belonging to class A over belonging to class B and the p-value of will tell you if there is any significant difference in the expected value of depending on whether something belongs to class A vs class B.

3.5 Extensions of the Linear Model

* Make models that include ***Interactions*** and ***Nonlinearity*** instead of relying on the assumption that the effect of the different parameters are additive.
* To account for interactions, you include ***Product terms*** between the different parameters:

Instead of an independent coefficient for the variable , the coefficient for is now modified to be ***dependent on the second variable*** . Now the value and p-value of the coefficient  ***gives you information about the strength and significance of the interaction***.

* Sometimes the interaction terms between variables are very significant (low p-value), but their main effects do not have strong significance (that is, there is a significant contribution of the interaction between and on the response variable , but the contribution of either or alone does not). In that case, it is custom to follow the ***Hierarchy Principle***:

*If we include an interaction in a model we should also include the main effects, even if the p-values associated with their coefficients are not significant.*

The reason that this is done is because it is usually difficult to interpret the model when you do not include the main effects. Specifically, ***the*** ***interaction terms also contain main effects if there are no main effect terms added to the model***.

* Models can be modified in the following way to include ***interactions between a*** ***quantitative and a qualitative variable*** in the following way:

In this case where there is ***no interaction*** between the classes and the variables, ***only the intercept*** will be different depending on whether the datapoint belongs to class A or class B.

In this case where ***there is an interaction*** between the classes and the variables, ***both the intercept and the slope*** can be different depending on whether the datapoint belongs to class A or class B.

* The same approach can be used to accommodate ***polynomials*** in the model:

In this case the model is still called a ***linear model*** (and so we still do linear regression), because the model is still linear in the coefficients.

**Chapter 4: Classification**

4.1 Introduction to Classification Problems

* Qualitative variables have values from an ***unordered set***.
* The task of the classification function is to take the values from and predict their qualitative values such that it assigns them to a specific class in the set.
* Typically, the major interest will be to ***estimate the*** ***probabilities that belongs to each category***.
* Can linear regression be used for a classification task?
* In the case of a binary outcome, linear regression can do quite well when implemented as follows:

You can then simply perform a linear regression of on and classify as **yes** when  .

* In addition, in this example of a binary outcome, in the population we have , which would be a further justification for the use of linear regression.
* In this case linear regression is equivalent to ***Linear Discriminant Analysis***.
* However, linear regression can produce probabilities that are ***Lower than zero and larger than one***. For this reason, ***Logistic Regression*** is more appropriate.
* When the variable can be classified into ***more than two categories*** then assigning values to the categories does not work, as it suggests an ***ordering*** between them. For example, when modelling the response as:

This implies that the difference between A and B is the same as between B and C, but not the same as the difference between A and C.

* For this case of a variable that can be classified into more than two categories, ***Linear Regression is not appropriate***.
* Instead, ***Multiclass Logistic Regression*** or ***Discriminant Analysis*** are more appropriate.

4.2 Logistic Regression

* ***Logistic Regression*** equation takes the following form:

This equation will always take on values ***between 0 and 1***, as is required for a probability.

* The equation can be rewritten to:

This shows that the equation for logistic regression still entails a ***linear model, but with the probabilities modelled on a non-linear scale***.

* To estimate the parameters when the different observations are independent of each other, we use ***maximum likelihood***:

This likelihood gives the probability of having the number of zeros and ones that we see in the data. For example, if the series of zeros and ones look like 1101001, then the above equation would calculate , where is the probability of having a one and is the probability of having a zero. The parameters and are chosen such that ***the likelihood of the observed data is maximized***.

* From fitting a logistic regression model, you can get the ***Z-statistic*** of the values that were found for the parameters. The Z-statistic shows a sort of standardized value for the parameters. For example, the value of the slope of the model will depend on the units that are used, and the Z-statistic corrects for that. In that way it gives a better view of how strong the relation is between the variables and the response.

4.3 Multivariate Logistic Regression

* Logistic regression with multiple variables takes the form:

Or, to have it in a form that is linear with respect to the variables:

* This can be used in a similar way as for linear regression to estimate the variables. Remember that some of these variables can be strongly correlated, which can make it more difficult to interpret their effect on the response (it can change depending on which other variables are present).

4.4 Logistic Regression - Case-Control Sampling and Multiclass

* ***Case Control Sampling*** is a popular tool in epidemiology because it allows to correct for a difference in the sampled cases compared to the actual number of cases in a population (For example, the prevalence of a disease may be 35% in the sampled population, while it is 5% in the actual population).
* With logistic regression and case control, you can still accurately estimate the regression parameters of interest (these are the slopes of the different variables , excluding the intercept ).
* The estimated value of will initially be incorrect, but can be corrected after fitting the logistic model using this transformation:

Where is the prevalence of cases in the actual population and is the prevalence of cases in the sampled population.

* Thus, with case control sampling you can estimate the parameters ***without requiring a large sample population*** (which is particularly a problem if the occurrence of the event is rare) and ***without requiring a large amount of time*** to determine how often the event occurs. Instead, you only need to take a small sample population of the controls (cases where the event did not happen) and compare it to a sample population where the event did happen.
* An example is the click through rate for ads. If you take a random subset of subjects that have been exposed to ads, you will have a large amount of 0’s (people that do not click) and only a few 1’s (people that do click). ***In case control, you do not use all this data to fit your model, but only take a sample of the controls, which will still give accurate estimates for the main parameters of the model when you make the fit.***
* When using case control, ***there is a trade-off between control:case ratio and the variance in the estimate of the parameters.*** When the ratio of control:case ratio reaches a value of around 5:1 to 6:1, the variance starts to flatten out, so at this threshold increasing the number of controls relative to the number of cases no longer significantly increases the accuracy if the estimated parameters.
* Logistic regression can be easily ***generalized to a situation where there are more than two classes***. One version used in R has the following symmetric form:

Where is one of the classes in the total set of classes. Here, you sum over the different linear functions for each class and you weigh the exponential term for class against this sum. This multiclass logistic regression is also known as ***Multinomial Regression***.

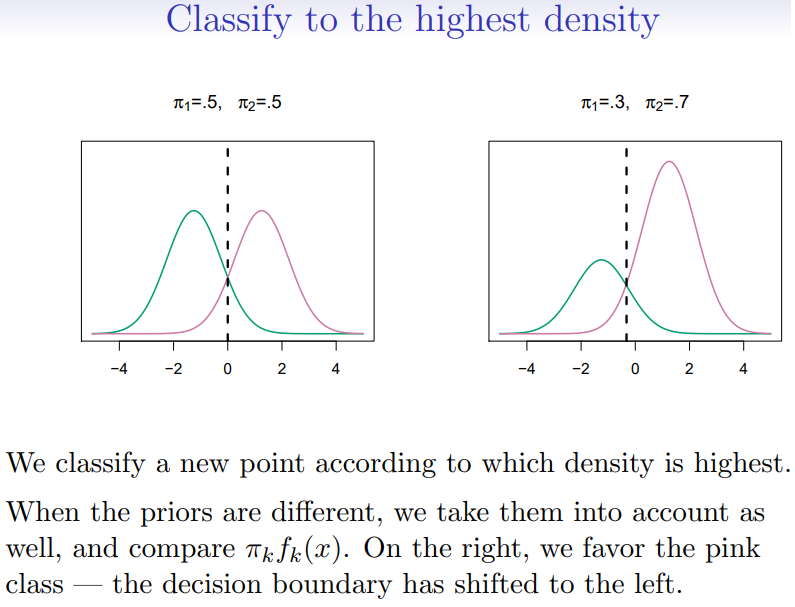
4.5 Discriminant Analysis

* In ***Discriminant Analysis*** the approach is to model the distribution of in each of the classes separately and then use ***Bayes theorem*** to find
* When each class is modelled using ***Normal/Gaussian distributions***, this leads to ***Linear or Quadratic Discriminant Analysis***.
* ***Bayes Theorem*** states:

For discriminant analysis, this is written as:

Here,is the (***Probability) Density for in class k***. is the ***Marginal or Prior probability for class k.***

* In discriminant analysis, points are basically classified ***according to which density is highest***. The ***decision boundary*** is the point at which the densities for the different classes intersect.

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* Discriminant analysis provides an ***advantage over Logistic Regression when the classes are well-separated***, in which case the parameter estimates from logistic regression can be unstable (coefficients can go to infinity when classes are perfectly separated). Linear discriminant analysis does not suffer from this problem.
* The linear discriminant model is also more stable than logistic regression when ***the sample size is small and the distribution of the predictors is approximately normal in each of the classes***.
* When there are ***more than 2 classes***, linear discriminant analysis gives a nice low-dimension view of the data.

4.6 Gaussian Discriminant Analysis – One Variable

* The Gaussian probability density function is:

Where is the distribution mean and is the variance (in class ). The part that ***makes the probability dependent on is in the exponential***.

* Whether the ***variance is the same in all classes*** (that is, , where is the variance in each class) ***will determine if discriminant analysis gives linear or quadratic functions***.
* Inserting the equation for a Gaussian function (assuming that ) into ***Bayes theorem*** gives:
* To classify an observation to a class, you initially don´t need to evaluate the probabilities, ***you simply need to see which of them is the largest***. By taking the logs and discarding the terms that do not depend on , you can see that this is equivalent to assigning to the class with the largest ***Discriminant Score***:

Where is a linear function of .

* To get the parameters of the Gaussian distribution (such as and ) from real data, you will need to estimate them from your dataset. These estimates are calculated as follows:

When the variance in all classes is the same (), you can use:

Here, is the number of observations of class and is the total number of observations.

4.7 Gaussian Discriminant Analysis-Many variables

* When there is a ***correlation*** between the different variables of the model, the Gaussian probability density function ***will become stretched*** as compared to a model where the variables are uncorrelated (in that case, the Gaussian probability density function looks like a Bell function).
* To extend Linear discriminant analysis from one variable to many variables, you need to use the ***Covariance Matrix*** in the formula for that was set-up for the single variable linear discriminant analysis.
* If you would know the true probability densities for the different classes, you would be able to determine the ***Bayes Decision Boundaries***. These are the decision boundaries that would give the ***fewest misclassification errors, among all possible classifiers***.
* Linear discriminant analysis ***classifies datapoints to the closest centroid***, which means that if there are classes, linear discriminant analysis can be viewed in exactly a dimensional plot.
* If the number of variables becomes ***very large*** (if you have variables, the covariance matrix will have size by ), you need to make other modifications to use discriminant analysis.
* If you have estimates for , then these estimates can be turned into estimates for the ***Class Probabilities***:

So classifying to the largest is the same as classifying to the class for which is largest.

* This also shows that linear discriminant analysis does not only give us the class to which an observation was classified, it also gives us ***the probability*** ***that observation belongs to class*** .
* The misclassification rate can be assessed using a ***Confusion Matrix***.
* The misclassification rate should be compared to the ***Null Rate*** to see how well the classification actually is. The null rate corresponds to the misclassification rate that is obtained when you ***always classify to the prior*** (that is, you classify to the largest class).
* The ***ROC Curve*** can be used to simultaneously plot both the ***False positive and the True positive rates***.
* The ***Area Under Curve (AUC)*** of the ROC curve to summarize how well the classification is performed (higher AUC is better). It tells you how close you are to a true positive rate of 1 and a false positive rate of 0.