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Labs

Lab 1

Assignment 1 – Logistic regression and KNN-method

#1: Read data and divide into test and train sets

```
Dataframe=read.csv2("spambase.csv")
n=dim(Dataframe)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=Dataframe[id,]
test=Dataframe[-id,]
```

#2: Use logistic regression (functions glm(), predict()) to classify the training and test data by the classification $\hat{Y} = 1$ if $p(Y=1 | X) > 0.5$, otherwise $\hat{Y}=0$ and report the confusion matrices (use table()) and the misclassification rates for training and test data. Analyse the obtained results.

```
#Create model for prediction
spammodel = glm(Spam~., family='binomial', data=train)
summary(spammodel)

#Predict values and create confusion matrix for traindata
predicted_values_train = predict(spammodel, newdata=train, type='response')
confusion_matrix_train = table(train$Spam, predicted_values_train>0.5)
print(confusion_matrix_train)

#Predict values and create confusion matrix for testdata
predicted_values_test = predict(spammodel, newdata=test, type='response')
confusion_matrix_test = table(test$Spam, predicted_values_test>0.5)
print(confusion_matrix_test)

#Create function for misclassification rate
missclass=function(conf_matrix, fit_matrix){
  n=length(fit_matrix[,1])
  return(1-sum(diag(conf_matrix))/n)
}

#Calculate misclassification rate for train and test data
missclass_train = missclass(confusion_matrix_train, train)
print(missclass_train)
missclass_test = missclass(confusion_matrix_test, test)
print(missclass_test)
```

#Conclusion: It is reasonable that the model performs better on the train data compared to the test data. However, the fact that the miscalculations are similar indicates that the model performs similarly on two different data sets which is generally how you want your model to behave. By analyzing the confusion matrices, it is notable that the model is wrong more times proportionally when trying to classify an email that is spam than an email that is not spam.

#3: Use logistic regression to classify the test data by the classification principle: Same as above but with threshold 0.8. Compare the results. What effect did the new rule have.

```
#Create confusion matrix where classification is based on threshold 0.8
confusion_matrix_train2 = table(train$Spam, predicted_values_train>0.8)
confusion_matrix_test2 = table(test$Spam, predicted_values_test>0.8)
print(confusion_matrix_train2)
print(confusion_matrix_test2)
```

```
#Calculate missclassification rate for train and test data with threshold 0.8
missclass_train2 = missclass(confusion_matrix_train2, test)
print(missclass_train2)
missclass_test2 = missclass(confusion_matrix_test2, train)
print(missclass_test2)
```

#Conclusion: The misclassification rates have similar results. Showing us that model is well fitted, since the model acts similar between trained and tested data. Although this classification principle gives us a higher misclassification rate, it lowered the risk of a non-spam being classified as spam substantially. Therefore we prefer this principle over the previous.

#4: Use standard classifier kknn() with K=30 from package kknn, report the misclassification rates for the training and test data and compare the results with step 2.

```
#Fetch package kkm
#install.packages("kknn")
library("kknn")

#Classify according to kknn with k=30 for test and train data sets
kknn_30_train = kknn(formula = Spam~., train, train, k=30)
kknn_30_test = kknn(formula = Spam~., train, test, k=30)
confusion_matrix_kknn30_train = table(train$Spam, kknn_30_train$fitted.values>0.5)
missclass_kknn30_train = missclass(confusion_matrix_kknn30_train, train)
confusion_matrix_kknn30_test = table(test$Spam, kknn_30_test$fitted.values>0.5)
missclass_kknn30_test = missclass(confusion_matrix_kknn30_test, test)
print(confusion_matrix_kknn30_train)
print(missclass_kknn30_train)
print(confusion_matrix_kknn30_test)
print(missclass_kknn30_test)
```

#Conclusion: The misclassification values between predictions of the different sets differ alot. This shows us that our model is not well fitted. The misclassification is lower for the trained data, since the model is fitted after these values. Compared to the results from using logistic regression to classify the data, the results from the KKN model were significantly worse on the test data. This implies that KKN classification with K=30 is worse than logistic regression in this case.

#5: Repeat step 4 for K=1. Classify according to kknn with k=1 for test and train data sets. What does the decrease of K lead to and why?

```
kknn_1_train = kknn(formula = Spam~., train, train, k=1)
kknn_1_test = kknn(formula = Spam~., train, test, k=1)
confusion_matrix_kknn1_train = table(train$Spam, kknn_1_train$fitted.values>0.5)
```

```

missclass_kknn1_train = missclass(confusion_matrix_kknn1_train, train)
confusion_matrix_kknn1_test = table(test$Spam, kknn_1_test$fitted.values>0.5)
missclass_kknn1_test = missclass(confusion_matrix_kknn1_test, test)
print(confusion_matrix_kknn1_train)
print(missclass_kknn1_train)
print(confusion_matrix_kknn1_test)
print(missclass_kknn1_test)

```

#Conclusion: The misclassification rate for the training confusion matrix is zero since it compares each data point to itself, predicting all correct. This explains the high misclassification rate for the confusion matrix made on the test data. Using K=1 is a very unreliable method because it does not imply a large statistical advantage.

Assignment 2 – Probabilistic model and Bayesian model (max.likelihood computations)

#1: Import data

```
Dataframe=read.csv2("machines_csv.csv")
```

#2: Assume probability model $p(x|\theta) = \theta \cdot e^{(-\theta \cdot x)}$ for $x = \text{Length}$ in which observations are independent and identically distributed. What is the distribution type of x . Write a function that computes the log-likelihood $\log p(x|\theta)$ for a given θ and a given data vector x . Plot the curve showing the dependence of log-likelihood on θ where the entire data is used for fitting. What is the maximum likelihood value of θ according to plot?

```
#Compute a function for calculating the maximum likelihood of a function
```

```
loglikelihood=function(theta, x){
  n = length(x[,1])
  return(n*log(theta)-theta*sum(x))
}
```

```
#Plot curve for different theta values
```

```
theta_curve = curve(-loglikelihood(x, Dataframe), xlab="Theta", from=min(Dataframe), to=max(Dataframe))
```

```
#Find maximum likelihood value of theta
```

```
theta_max = function(x){
  n=length(x[,1])
  return(n/sum(x))
}
```

```
#Find maxtheta
```

```
max_theta = theta_max(Dataframe)
print(max_theta)
```

#Conclusion: We can see from the probabilistic model that the distribution is of type exponential. The maximum likelihood value of θ is: 42.29453 The optimal θ for is: 1.126217

#3: Repeat step 2 but use only 6 first observations from the data, and put the two log-likelihood curves (from step 2 and 3) in the same plot. What can you say about reliability of the maximum likelihood solution in each case?

```
#New vector with first 6 values
```

```
y = matrix(Dataframe[1:6,1], nrow=length(Dataframe[1:6,1]), ncol=1)
print(y)
```

```
#Plot new curve on top of each other
```

```
curve(-loglikelihood(x, Dataframe), xlab="Theta", from=0, to=20, add=FALSE, col="red", ylim=c(0,100))
curve(-loglikelihood(x, y), xlab="Theta", from=0, to=20, add=TRUE, col="blue", ylim=c(0,100))
```

#Conclusion: The graph is increasing at a much slower pace when only using the first six values compared with to the graph when we use all data. The model with more data is more reliable since there is a more certain min-value from the graph whereas the one with only six values, the theta value could be anything from the minimum value and forward.

#4: Assume now a Bayesian model with $p(x|\theta)=\theta \cdot e^{(-\theta \cdot x)}$ and a prior $p(\theta)=\lambda \cdot e^{(-\lambda \cdot \theta)}$, $\lambda=10$. Write a function computing $l(\theta)=\log(p(x|\theta) \cdot p(\theta))$. What kind of measure is actually computed by this function? Plot the curve showing the dependence of $l(\theta)$ on θ computed using the entire data and overlay it with a plot from step 2. Find an optimal θ and compare your result with the previous findings.

#Compute a function for calculating the likelihood of the bayesian function

```
bayesian_likelihood=function(theta, lambda, x){  
  n = length(x[,1])  
  return(n*log(theta)-theta*sum(x)-lambda*theta)  
}
```

#Find maximum likelihood value of theta

```
bayesian_theta_max = function(lambda, x){  
  n=length(x[,1])  
  return(n/(sum(x)+lambda))  
}
```

#Find maxtheta

```
bayesian_max_theta = bayesian_theta_max(10, Dataframe)  
print(bayesian_max_theta)
```

#Plot new curve on top of each other

```
curve(-bayesian_likelihood(x, 10, Dataframe), ylab="-Loglikelihood", xlab="Theta", from=0, to=10, add=FALSE,  
col="red", ylim=c(20,300))  
curve(-loglikelihood(x, Dataframe), ylab="-Loglikelihood", xlab="Theta", from=0, to=10, add=TRUE, col="blue",  
ylim=c(20,300))
```

#Conclusion: When using an bayesian model we have a prior that gives the model information beforehand which helps fitting the model. The optimal theta is now 0.91 which is close to the datasets meanvalue, which makes sense that this model gives a better predicted value.

#5: Use theta value found in step 2 and generate 50 new observations from $p(x|\theta)=\theta \cdot e^{(-\theta \cdot x)}$ (use standard number generators). Create the histograms of the original and the new data and make conclusions.

#Generate 50 new observation using theta value from step 2

```
set.seed(12345)  
newdata = rexp(50, rate = max_theta)  
print(newdata)
```

#Plot new data and old data in histogram

```
olddata = Dataframe$Length  
print(olddata)  
hist(newdata)  
hist(olddata)
```

#Conclusion: The histogram shows us that the distribution is fairly similar between the actual and predicted data. This concludes model was accurately fitted to the correct distribution model.

Assignment 4 – Linear regression, Ridge, LASSO, stepAIC

#1: Read data and plot Moisture vs Protein

```
Dataframe=read.csv2("tecator_csv.csv")
n = length(Dataframe[,1])
print(Dataframe)
moisture = Dataframe$Moisture
protein = Dataframe$Protein
fat = Dataframe$Fat
plot(moisture, protein, type="p", ylab="Protein", xlab="Moisture", col="red")
```

#Conclusion: Looks like a linear relation so a linear regression model is appropriate

#2: Consider model M_i in which Moisture is normally distributed, and the expected Moisture is a polynomial function of Protein including the polynomial terms up to power of i (i.e. M_1 is a linear model, M_2 is a quadratic model and so on). Report a probabilistic model that describes M_i . Why is it appropriate to use MSE criterion when fitting this model to a training data?

#Conclusion: A probabilistic model describing $M(i)$ is: $M(i) = w_0 + w_1 * X + w_2 * X^2 + \dots + w_i * X^i$ (3) The MSE criterion is a suitable method since it punishes outliers to a larger extent. This creates a better fitted model compared to when you punish the absolute value. This reduces the risk of an overfitted model.

#3: Divide the data into training and validation sets (50%/50%) and fit models M_i , $i=1,\dots,6$. For each model, record the training and the validation MSE and present a plot showing how training and validation MSE depend on i (write some R code to make this plot). Which model is best according to the plot? How do the MSE values change and why? Interpret this picture in terms of bias-variance tradeoff.

```
colno_protein = which(colnames(Dataframe)=="Protein")
colno_moisture = which(colnames(Dataframe)=="Moisture")
moisture_protein = Dataframe[colno_protein:colno_moisture]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=Dataframe[id,]
test=Dataframe[-id,]
moisture_train = train$Moisture
moisture_test = test$Moisture

#Create function for fitting linear regression models
fit_moisture_model = function(x) {
  return(lm(formula = Moisture ~ poly(Protein, degree=x), data=train))
}
```

```
#Create predict function for training set
predict_train = function(model){
  return(predict(model, newdata = train))
}
```

```
#Create predict function for test set
predict_test = function(model){
  return(predict(model, newdata = test))
}
```

```
#Create function for calculating MSE, input parameters are vectors containing original data and predicted data
calcMSE = function(y, yhat){
  return(sum((y-yhat)^2)/length(y))
}
```

#Create models and predictions and store MSE values in a vector for training and test data

```

vector_train = c()
vector_test = c()
for (i in 1:6){
  fit = fit_moisture_model(i)
  predicted_train = predict_train(fit)
  predicted_test = predict_test(fit)
  vector_train[i] = calcMSE(moisture_train, predicted_train)
  vector_test[i] = calcMSE(moisture_test, predicted_test)
}

#Create numeric vector 1 through 6
models = c(1:6)

#Plot MSE for each model
plot(models, vector_train, col="blue", xlab="Model", ylab="MSE")
par(new=TRUE)
plot(models, vector_test, col="red", xlab="Model", ylab="MSE")

#Print MSE values
print(vector_train)
print(vector_test)

```

#Conclusion: Shown in the graphs we can see that for the tested values, M(3) has the lowest MSE and therefore being the model with the smallest error. In terms of bias, what we can see is that in the training model the predicted error, and MSE, is descending for a more complex model, because bias is defined by the ability for a model to fit data. This gives us an overfitted model, where we can see that the variance increases the more complex models because the MSE increases for the tested data and the MSE decreases for the training data. Variance is defined by the difference in predictions on different data sets.

#Use the entire data set in the following computations:

#4: Fat response and Channel1-100 are predictors. Use stepAIC. How many variables were selected?

```

#Fetch package stepAIC
#install.packages("MASS")
library("MASS")

#Perform stepAIC on fat
colno_fat = which(colnames(Dataframe)=="Fat")
channel_values = Dataframe[1:(colno_fat-1)]
fit_fat = lm(fat~., data = channel_values)
step = stepAIC(fit_fat, direction="both")
step$anova
summary(step)

```

#Conclusion: When we use StepAIC in total 63 variables were selected. These were chosen because not all variables are needed to predict a dependent variable.

#5: Fit a Ridge regression model with same predictor and response variables. Plot model coefficient depend on the log of the penalty factor lambda and report how the coefficients change with lambda.

```

#install.packages("glmnet")
library("glmnet")
covariates = scale(Dataframe[,2:(colno_fat-1)])
response = scale(Dataframe[,colno_fat])
ridge_model = glmnet(as.matrix(covariates), response, alpha=0, family="gaussian")
plot(ridge_model, xvar="lambda", label=TRUE)

```

#Coefficients goes towards 0 when lambda goes towards infinity

#6: Repeat last step but with LASSO instead of Ridge. Differences?

```
lasso_model = glmnet(as.matrix(covariates), response, alpha=1, family="gaussian")
plot(lasso_model, xvar="lambda", label=TRUE)
```

#Conclusion 5 and 6: The graphs below shows us that when we increase lambda fewer variables are selected to the models, since the coefficients goes towards zero. In the Lasso model, the penalty is the absolute value, and in the Ridge model the penalty is squared (penalizes large values more).

#7: Choose the best model by cross validation for LASSO model. Report optimal lambda and how many variables that chosen by the model and make conclusions. Present also a plot showing the dependence of the CV score and comment how the CV score changes with lambda.

```
lasso_model_optimal = cv.glmnet(as.matrix(covariates), response, alpha=1, family="gaussian",
lambda=seq(0,1,0.001))
lasso_model_optimal$lambda.min
plot(lasso_model_optimal)
coef(lasso_model_optimal, s="lambda.min")
print(lasso_model_optimal$lambda.min)
```

#Conclusion: When the lambda increases in value, the MSE seems to strictly increase. From this model, we can make the conclusion that the optimal lambda = 0. This means, that all variables should be included for a better predicted model. Compared to the results from stepAIC, all variables were chosen since lambda = 0 instead of 63 that were chosen.

Lab 2

Assignment 1 - LDA and logistic regression. Draw decision boundary

#1: Read data and plot carapace length versus rear width (obs coloured by sex). Do you think that this data is easy to classify by LDA? Motivate answer.

```
RNGversion('3.5.1')
Dataframe=read.csv("australian-crabs.csv")
n = length(Dataframe[,1])
CL = Dataframe$CL
RW = Dataframe$RW
plot(CL, RW, main="Plot of carapace length versus rear width depending on sex", sub="Red = Female, Blue = Male",
col=c("red", "blue")[Dataframe$sex], xlab="CL", ylab="RW")
```

#Conclusion:

```
#Create function for misclassification rate
missclass=function(conf_matrix, fit_matrix){
  n=length(fit_matrix[,1])
  return(1-sum(diag(conf_matrix))/n)
}
```

#2: LDA analysis with target Sex, and features CL and RW and proportional prior by using lda() function in package MASS Make a Scatter plot of CL versus RW colored by the predicted Sex and compare it with the plot in step 1. Compute the misclassification error and comment on the quality of fit.

```
library("MASS")
```



```

model = lda(sex ~ CL+RW, data=Dataframe)
predicted = predict(model, data=Dataframe)
confusion_matrix = table(Dataframe$sex, predicted$class)
misclass = missclass(confusion_matrix, Dataframe)
print(confusion_matrix)
print(misclass)
plot(CL, RW, main="Plot predicted values of CL and RW depending on sex", sub="Red = Female, Blue = Male",
     col=c("red", "blue")[predicted$class], xlab="CL", ylab="RW")

```

#3: Repeat step 2 but use priors $p(\text{Male})=0.9$ and $p(\text{Female})=0.1$

```

model2 = lda(sex ~ CL+RW, data=Dataframe, prior=c(1,9)/10)
predicted2 = predict(model2, data=Dataframe)
confusion_matrix2 = table(Dataframe$sex, predicted2$class)
misclass2 = missclass(confusion_matrix2, Dataframe)
print(confusion_matrix2)
print(misclass2)
plot(CL, RW, main="Plot predicted values of CL and RW with priors  $p(\text{Male})=0.9$  and  $p(\text{Female})=0.1$ ",
     sub="Red = Female, Blue = Male", col=c("red", "blue")[predicted2$class], xlab="CL", ylab="RW")

```

#4: Repeat step 2 but now with logistic regression (use function `glm()`). Compare with LDA results. Finally, report the equation of the decision boundary and draw the decision boundary in the plot of the classified data.

```

model3 = glm(sex ~ CL+RW, data=Dataframe, family='binomial')
predicted3 = predict(model3, newdata=Dataframe, type='response')
sexvector = c()
for (i in predicted3) {
  if (i>0.9) {
    sexvector = c(sexvector, 'Male')
  } else {
    sexvector = c(sexvector, 'Female')
  }
}
print(sexvector)
sexvector_factor = as.factor(sexvector)
confusion_matrix3 = table(Dataframe$sex, sexvector_factor)
misclass3 = missclass(confusion_matrix3, Dataframe)
print(confusion_matrix3)
print(misclass3)
plot(CL, RW, main="Plot predicted values of CL and RW but with logistic regression",
     col=c("red", "blue")[sexvector_factor], xlab="CL", ylab="RW", xlim=c(0,50), ylim=c(0,20))

boundaryline = function(length, coefficientvector, prior) {
  return(-coefficientvector[1]/coefficientvector[3]-
  (coefficientvector[2]/coefficientvector[3])*length+log(prior/(1-prior))/coefficientvector[3])
}
par(new=TRUE)
curve(boundaryline(x, model3$coefficients, 0.9), xlab="CL", ylab="RW", col="green", from=0, to=50,
      xlim=c(0,50), ylim=c(0,20),
      sub="Red = Female, Blue = Male, Green = Boundaryline")

```

Assignment 2 – Split method, Tree modeling (gini and deviance), Naïve Bayes, loss matrix

#1: Read data and divide into train, validation and test sets as 50/25/25.

```

library("tree")

```

```
RNGversion('3.5.1')
```

```
data=read.csv2("creditscoring.csv")
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]
id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.25))
valid=data[id2,]
id3=setdiff(id1,id2)
test=data[id3,]
```

```
#Create function for misclassification rate
misclass=function(conf_matrix, fit_matrix){
  n=length(fit_matrix[,1])
  return(1-sum(diag(conf_matrix))/n)
}
```

#2: Fit a decision tree to train data using the measures of impurity gini and deviance. Report misclass rates and choose optimal measure moving forward.

```
fit_deviance=tree(good_bad~., data=train, split="deviance")
predicted_deviance=predict(fit_deviance, newdata=test, type="class")
confusionmatrix_deviance=table(test$good_bad, predicted_deviance)
misclass_deviance=misclass(confusionmatrix_deviance, test)
print(confusionmatrix_deviance)
print(misclass_deviance)
fit_gini=tree(good_bad~., data=train, split="gini")
predicted_gini=predict(fit_gini, newdata=test, type="class")
confusionmatrix_gini=table(test$good_bad, predicted_gini)
misclass_gini=misclass(confusionmatrix_gini, test)
print(confusionmatrix_gini)
print(misclass_gini)
#Deviance has best misclass score
```

#3: Use training and valid data to choose optimal tree depth. Present graphs of the dependence of deviances for training and validation data on the number of leaves. Report optimal tree, report it's depth and variables used by tree. Estimate misclassification rate for the test data.

```
fit_optimaltree=tree(good_bad~., data=train, split="deviance")
summary(fit_optimaltree)
trainScore=rep(0,15)
testScore=rep(0,15)
for(i in 2:15){
  prunedTree=prune.tree(fit_optimaltree, best=i)
  pred=predict(prunedTree, newdata=valid, type="tree")
  #Divide by two since double of data points
  trainScore[i]=deviance(prunedTree)/2
  testScore[i]=deviance(pred)
}
plot(2:15, trainScore[2:15], type="b", col="red", ylim=c(200,500))
points(2:15, testScore[2:15], type="b", col="blue")
min_deviance=min(testScore[2:15])
print(min_deviance)
optimal_leaves=which(testScore[1:15] == min_deviance)
```

```

print(optimal_leaves)
#Optimal no of leaves is 4
finalTree=prune.tree(fit_optimaltree, best=4)
summary(finalTree)
plot(finalTree)
text(finalTree, pretty=0)

```

#Final tree contains variables savings, duration and history. Since 3 vars => Depth of tree is 3.

```

predicted_test=predict(finalTree, newdata=test, type="class")
confusionmatrix_test=table(test$good_bad, predicted_test)
misclass_test=misclass(confusionmatrix_test, test)
print(confusionmatrix_test)
print(misclass_test)

```

#4: Use training data to perform classification using Naives bayes and report the confusion matrices and misclassification rates for the training and for the test data. Compare with results from previous steps.

```

#Load libraries
library(MASS)
library(e1071)
fit_naive=naiveBayes(good_bad~., data=train)
#Create function for predicting and creating confusion matrix and printing misclassification rate
compute_naive=function(model,data){
  predictedNaive=predict(model, newdata=data, type="class")
  confusionmatrixNaive=table(data$good_bad,predictedNaive)
  misclass = misclass(confusionmatrixNaive, data)
  print(confusionmatrixNaive)
  print(misclass)
  return(predictedNaive)
}
predictedNaive_train=compute_naive(fit_naive,train)
predictedNaive_test=compute_naive(fit_naive, test)

```

#5: Use optimal tree and Naives Bayes to classify the test data by using principle: classified as 1 if 'good' bigger than 0.05, 0.1, 0.15, ..., 0.9, 0.95. Compute the TPR and FPR for two models and plot corresponding ROC curves.

```

#Writing function for classifying data
class=function(data, class1, class2, prior){
  vector=c()
  for(i in data) {
    if(i>prior){
      vector=c(vector,class1)
    } else {
      vector=c(vector,class2)
    }
  }
  return(vector)
}

```

```

x_vector=seq(0.05,0.95,0.05)
tpr_tree=c()
fpr_tree=c()
tpr_naive=c()
fpr_naive=c()
treeVector=c()

```

```

treeConfusion = c()
naiveConfusion = c()
treeClass = c()
naiveClass = c()
#Reusing optimal tree found in task 3 but returntype is response instead
set.seed(12345)
predictTree=data.frame(predict(finalTree, newdata=test, type="vector"))
predictNaive=data.frame(predict(fit_naive, newdata=test, type="raw"))
for(prior in x_vector){
  treeClass = class(predictTree$good, 'good', 'bad', prior)
  treeConfusion=table(test$good_bad, treeClass)
  if(ncol(treeConfusion)==1){
    if(colnames(treeConfusion)=="good"){
      treeConfusion=cbind(c(0,0), treeConfusion)
    } else {
      treeConfusion=cbind(treeConfusion,c(0,0))
    }
  }
  totGood=sum(treeConfusion[2,])
  totBad=sum(treeConfusion[1,])
  tpr_tree=c(tpr_tree, treeConfusion[2,2]/totGood)
  fpr_tree=c(fpr_tree, treeConfusion[1,2]/totBad)
  print(fpr_tree)
  naiveClass=class(predictNaive$good, 'good', 'bad', prior)
  naiveConfusion=table(test$good_bad, naiveClass)
  if(ncol(naiveConfusion)==1){
    if(colnames(naiveConfusion)=="good"){
      naiveConfusion=cbind(c(0,0), naiveConfusion)
    } else {
      naiveConfusion=cbind(naiveConfusion,c(0,0))
    }
  }
  totGood=sum(naiveConfusion[2,])
  totBad=sum(naiveConfusion[1,])
  tpr_naive=c(tpr_naive, naiveConfusion[2,2]/totGood)
  fpr_naive=c(fpr_naive, naiveConfusion[1,2]/totBad)
}
#Plot the ROC curves
plot(fpr_naive, tpr_naive, main="ROC curve", sub="Red = Naive Bayes, Blue = Tree", type="l", col="red",
xlim=c(0,1),
ylim=c(0,1), xlab="FPR", ylab="TPR")
points(fpr_tree, tpr_tree, type="l", col="blue")

```

#Naive has greatest AOC => should choose Naive

#6: Repeat Naive Bayes with loss matrix punishing with factor 10 if predicting good when bad and 1 if predicting bad when good.

```

naiveModel=naiveBayes(good_bad~., data=train)
train_loss=predict(naiveModel, newdata=train, type="raw")
test_loss=predict(naiveModel, newdata=test, type="raw")
confusion_trainLoss=table(train$good_bad, ifelse(train_loss[,2]/train_loss[,1]>10, "good", "bad"))
misclass_trainLoss=misclass(confusion_trainLoss, train)
print(confusion_trainLoss)
print(misclass_trainLoss)
confusion_testLoss=table(test$good_bad, ifelse(test_loss[,2]/test_loss[,1]>10, "good", "bad"))
misclass_testLoss=misclass(confusion_testLoss, test)

```

```
print(confusion_testLoss)
print(misclass_testLoss)
```

#The misclassification rates have changed since a higher punishment is given when predicting good creditscore when in fact it was bad (reasonable since bank loses money then). It is less worse to predict bad creditscore but turns out to be good (just a loss of customer). Due to this more errors occur mainly because fewer people are classified to have good creditscores.

Assignment 4 – Principal components, PCA analysis, ICA analysis, Trace plots

```
#Read data
RNGversion('3.5.1')
```

```
data=read.csv2("NIRspectra.csv")
data$Viscosity=c()
n=dim(data)[1]
```

#1: Conduct standard PCA using the feature space and provide a plot explaining how much variation is explained by each feature. Provide plot that show the scores of PC1 vs PC2. Are there unusual diesel fuels according to this plot.

```
pcaAnalysis=prcomp(data)
lambda=pcaAnalysis$sdev^2
#Eigenvalues
print(lambda)
#Proportion of variation
propVar= lambda/sum(lambda)*100
screeplot(pcaAnalysis)
print(propVar)
noOfVars=1
sumOfVariation=propVar[noOfVars]
while(sumOfVariation<99){
  noOfVars=noOfVars+1
  sumOfVariation=sumOfVariation+propVar[noOfVars]
}
#Print number of variables used
print(noOfVars)
#Print PC1 and PC2 in plot
plot(pcaAnalysis$x[,1],pcaAnalysis$x[,2], ylim=c(-10,10), type="p", col="blue", main="PC1 vs PC2", xlab="PC1",
ylab="PC2")
#We can see from the graph that the data is very accurately described by PC1.
```

#2: Make trace plots of the loadings of the components selected in step 1. Is there any principle component that is explained by mainly a few original features?

```
U=pcaAnalysis$rotation
plot(U[,1], main="Traceplot, PC1", xlab="index", ylab="PC1", type="b")
plot(U[,2], main="Traceplot, PC2", xlab="index", ylab="PC2", type="b")
#We can see from graph that PC2 is not described by so many original features since it is close to zero for many of the features. The last 30 or so variables have an effect on PC2.
```

#3: Perform independent Component Analysis (ICA) with no of components selected in step1 (set seed 12345). Check the documentation of R for fastICA method and do following:

Compute $W'=K*W$ and present columns of W' in form of the trace plots. Compare with trace plots in step 2 and make conclusions. What kind of measure is represented by the matrix W' .

Make a plot of the scores of the first two latent features and compare it with the score plot from step 1.

```
#Install package fastICA
```

```
#install.packages("fastICA")
library("fastICA")

set.seed(12345)
icaModel = fastICA(data, n.comp=2, verbose=TRUE)
W=icaModel$W
K=icaModel$K
W_est=K%*%W
plot(W_est[,1], main="Traceplot, ICA1", xlab="index", ylab="ICA1", type="b", col="red")
plot(W_est[,2], main="Traceplot, ICA2", xlab="index", ylab="ICA2", type="b", col="red")
#Compared to the plots in step 2 the ICA1 follows in roughly the same pattern as PCA2 and ICA2 the same as PCA1.
```

```
plot(icaModel$S[,1], icaModel$S[,2], main="ICA1 vs ICA2", xlab="ICA1", ylab="ICA2", type="p", col="blue")
```

#We can see from the plot that the data is pretty well described by ICA2 whereas ICA1 is not that significant in describing the data (since it is close to 0 most of the cases). Some outliers are however described by ICA1.

Lab 3

Assignment 1 – Kernel methods, Smoothing coefficients

```
RNGversion('3.5.1')
```

Assignment 1:

Implement a kernel method to predict the hourly temperatures for a date and place in Sweden.

To do so, you are provided with the files stations.csv and temps50k.csv. These

files contain information about weather stations and temperature measurements in the stations

at different days and times. The data have been kindly provided by the Swedish Meteorological

and Hydrological Institute (SMHI).

You are asked to provide a temperature forecast for a date and place in Sweden. The

forecast should consist of the predicted temperatures from 4 am to 24 pm in an interval of 2

hours. Use a kernel that is the sum of three Gaussian kernels:

The first to account for the distance from a station to the point of interest.

The second to account for the distance between the day a temperature measurement

was made and the day of interest.

The third to account for the distance between the hour of the day a temperature measurement

was made and the hour of interest.

Choose an appropriate smoothing coefficient or width for each of the three kernels above.

Answer to the following questions:

Show that your choice for the kernels' width is sensible, i.e. that it gives more weight

to closer points. Discuss why your definition of closeness is reasonable.

Instead of combining the three kernels into one by summing them up, multiply them.

Compare the results obtained in both cases and elaborate on why they may differ.

Note that the file temps50k.csv may contain temperature measurements that are posterior

to the day and hour of your forecast. You must filter such measurements out, i.e. they cannot

be used to compute the forecast. Feel free to use the template below to solve the assignment.

```
set.seed(1234567890)
#install.packages("geosphere")
library(geosphere)
stations <- read.csv("stations.csv")
temps <- read.csv("temps50k.csv")
#A join operation on "station_number"
st <- merge(stations, temps, by="station_number")
n = dim(st)[1]
#Kernel weighting factors
h_distance <- 100000
h_date <- 20
```

```

h_time <- 2
#Latitude of interest
a <- 59.4059
#Longitude of interest
b <- 18.0256
#Coordinates for Danderyd
#Create a vector of the point of interest
placeOI = c(a, b)
dateOI <- as.Date("1995-07-29") # The date to predict (up to the students), my birth date
timesOI = c("04:00:00", "06:00:00", "08:00:00", "10:00:00", "12:00:00", "14:00:00", "16:00:00", "18:00:00",
"20:00:00",
"22:00:00", "24:00:00")

plotDist = function(dist, h){
  u = dist/h
  plot(dist, exp(-u^2), type="l", main="Plot of kernel wights for distances", xlab="Distance")
}

dist = seq(0, 100000, 1)
plotDist(dist, h_distance)

plotDate = function(date, h){
  u = date/h
  plot(date, exp(-u^2), type="l", main="Plot of kernel wights for dates", xlab="Days")
}

date = seq(-182,182,1)
plotDate(date, h_date)

plotTime = function(time, h){
  u = time/h
  plot(time, exp(-u^2), type="l", main="Plot of kernel wights for time", xlab="Hours")
}

time = seq(-12,12,1)
plotTime(time, h_time)

#Remove posterior data
filter_posterior = function(date, time, data){
  return(data[which(as.numeric(difftime(strptime(paste(date, time, sep=" "), format="%Y-%m-%d %H:%M:%S"),
strptime(paste(data$date, data$time, sep=" "),format="%Y-%m-%d %H:%M:%S"))))>0), 1])
}

#A gaussian function for the difference in distance
gaussian_dist = function(place, data, h) {
  lat = data$latitude
  long = data$longitude
  points = data.frame(lat,long)
  u = distHaversine(points, place)/h
  return (exp(-u^2))
}

xy = gaussian_dist(placeOI, st, h_distance)

#A gaussian function for difference in days
gaussian_day = function(date, data, h){
  compare_date = as.Date(data$date)

```

```

diff = as.numeric(date-compare_date)
for (i in 1:length(diff)) {
  if (diff[i] > 365) {
    diff[i] = diff[i] %% 365
    if(diff[i]>182){
      diff[i]=365-diff[i]
    }
  }
}
u = diff/h
return (exp(-u^2))
}

```

```

#A gaussian function for difference in hours
gaussian_hour = function(hour, data, h){
  compare_hour = strptime(data$time, format="%H:%M:%S")
  compare_hour = as.numeric(format(compare_hour, format="%H"))
  hour = strptime(hour, format="%H:%M:%S")
  hour = as.numeric(format(hour, format="%H"))
  diff = abs(hour-compare_hour)
  for (i in 1:length(diff)){
    if(diff[i]>12){
      diff[i] = 24-diff[i]
    }
  }
  u=diff/h
  return(exp(-u^2))
}

```

```

#Defining values that will be used in loop below
kernel_sum = c()
kernel_mult = c()

```

```

#Looping through time array and data points in nested loop to calculate the 11 kernel values
for (time in timesOI) {
  filtered_data = filter_posterior(dateOI, time, st)
  kernel_dist = gaussian_dist(placeOI, filtered_data, h_distance)
  kernel_day = gaussian_day(dateOI, filtered_data, h_date)
  kernel_time = gaussian_hour(time, filtered_data, h_time)
  sum_kernel = kernel_dist+kernel_day+kernel_time
  temp_sum = sum(sum_kernel * filtered_data$air_temperature)/sum(sum_kernel)
  mult_kernel = kernel_dist*kernel_day*kernel_time
  temp_mult = sum(mult_kernel * filtered_data$air_temperature)/sum(mult_kernel)
  kernel_sum = c(kernel_sum, temp_sum)
  kernel_mult = c(kernel_mult, temp_mult)
}

```

```

plot(kernel_sum, type="o", main="Temperature estimate through sum of factors", xlab="Time",
      ylab="Est. temperature")
axis(1, at=1:length(timesOI), labels=timesOI)
plot(kernel_mult, type="o", main="Temperature estimate through product of factors", xlab="Time",
      ylab="Est. temperature")
axis(1, at=1:length(timesOI), labels=(timesOI))

```


Assignment 2 – Support vector machines

##Support vector machines assignment

```
library(kernlab)
set.seed(1234567890)
data(spam)
```

```
#Create function for misclassification rate
missclass=function(conf_matrix, fit_matrix){
  n=length(fit_matrix[,1])
  return(1-sum(diag(conf_matrix))/n)
}
```

```
index=sample(1:4601)
train=spam[index[1:2500],]
valid=spam[index[2501:3501],]
test=spam[index[3502:4601],]
```

```
svmmodel1=ksvm(type~., data=train, kernel="rbfdot", kpar=list(sigma=0.05), C=0.5)
pred1=predict(svmmodel1, newdata=valid)
confusion1=table(valid$type, pred1)
misclass1=missclass(confusion1, valid)
print(confusion1)
print(misclass1)
```

```
svmmodel2=ksvm(type~., data=train, kernel="rbfdot", kpar=list(sigma=0.05), C=1)
pred2=predict(svmmodel2, newdata=valid)
confusion2=table(valid$type, pred2)
misclass2=missclass(confusion2, valid)
print(confusion2)
print(misclass2)
```

```
svmmodel3=ksvm(type~., data=train, kernel="rbfdot", kpar=list(sigma=0.05), C=5)
pred2=predict(svmmodel3, newdata=valid)
confusion3=table(valid$type, pred2)
misclass3=missclass(confusion3, valid)
print(confusion3)
print(misclass3)
```

##Answer: The model with the C value of 1 is the best since it has the lowest misclassification rate. However, since the application is classification of spam emails, the value of C=0.5 is the best since it classified the least nonspam emails as spam.

```
finalmodel=ksvm(type~., data=spam[index[1:3501],], kernel="rbfdot", kpar=list(sigma=0.05), C=1)
finalpred=predict(finalmodel, newdata=test)
finalconfusion=table(test$type, finalpred)
finalmisclass=missclass(finalconfusion, test)
print(finalconfusion)
print(finalmisclass)
```

##Answer: The purpose of the parameter C is to put a weight to the cost function. The higher C the more cost will a constraint violation yield.

Assignment 3 – Neural networks, weight initialization

Assignment3:

Train a neural network to learn the trigonometric sine function. To do so, sample 50 points

uniformly at random in the interval [0,10]. Apply the sine function to each point. The resulting
 ## pairs are the data available to you. Use 25 of the 50 points for training and the rest for validation.
 ## The validation set is used for early stop of the gradient descent. That is, you should
 ## use the validation set to detect when to stop the gradient descent and so avoid overfitting.
 ## Stop the gradient descent when the partial derivatives of the error function are below a given
 ## threshold value. Check the argument threshold in the documentation. Consider threshold
 ## values $i/1000$ with $i = 1, \dots, 10$. Initialize the weights of the neural network to random values in
 ## the interval [-1, 1]. Use a neural network with a single hidden layer of 10 units. Use the default values
 ## for the arguments not mentioned here. Choose the most appropriate value for
 ## the threshold. Motivate your choice. Provide the final neural network learned with the chosen
 ## threshold. Feel free to use the following template.

```
RNGversion('3.5.1')
#install.packages("neuralnet")
library(neuralnet)
set.seed(1234567890)
Var <- runif(50, 0, 10)
trva <- data.frame(Var, Sin=sin(Var))
train <- trva[1:25,] # Training
valid <- trva[26:50,] # Validation
n = dim(valid)[1]
# Random initialization of the weights in the interval [-1, 1]
winit <- runif(31, -1, 1)
trainScore = rep(0,10)
validScore = rep(0,10)
for(i in 1:10) {
  nn_temp <- neuralnet(Sin~Var, data=train, hidden=10, threshold=i/1000, startweights=winit)
  nn = as.data.frame(nn_temp$net.result)
  pred=predict(nn_temp, newdata=valid)
  trainScore[i] = 1/n*sum((nn[,1]-train$Sin)^2)
  validScore[i] = 1/n*sum((pred-valid$Sin)^2)
}
plot(1:10, trainScore[1:10], type="b", col="red", xlab="Threshold index", ylab="MSE")
points(1:10, validScore[1:10], type="b", col="blue")
min_error=min(validScore[1:10])
print(min_error)
optimal_i=which(validScore[1:10] == min_error)
print(optimal_i)
optimal_nn = neuralnet(Sin~Var, data=train, hidden=10, threshold=optimal_i/1000, startweights=winit)
plot(optimal_nn)
# Plot of the predictions (black dots) and the data (red dots)
plot(prediction(optimal_nn)$rep1)
points(trva, col = "red")
```

Exam

2018-01-11

Assignment 1 – PCA, PCA Regression, LDA, Tree

```
#Read data and divide randomly into train and test
Dataframe=read.csv("video.csv")
Dataframe$codec = c()
n=dim(Dataframe)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=Dataframe[id,]
```

```
test=Dataframe[-id,]
```

##Perform principle component analysis with and without scaling. How many vars for 95 % of variation in both cases. Explain why so few components are needed when scaling is not done.

```
PCAdata=subset(train, select=-utime)
pcaAnalysis_noScale=prcomp(PCAdata, scale=FALSE)
screeplot(pcaAnalysis_noScale)
lambda=pcaAnalysis_noScale$sdev^2
print(lambda)
#Proportion of variation
propVar=lambda/sum(lambda)*100
print(propVar)
#Function for calculating the number of components needed for explaining at least 95% of the variation.
calcNoVars = function(data){
  noOfVars=1
  sumOfVariation=data[noOfVars]
  while(sumOfVariation<95){
    noOfVars=noOfVars+1
    sumOfVariation=sumOfVariation+data[noOfVars]
  }
  return(noOfVars)
}
print(calcNoVars(propVar))
pcaAnalysis_scale=prcomp(PCAdata, scale=TRUE)
lambda_scale=pcaAnalysis_scale$sdev^2
propVar_scale=lambda_scale/sum(lambda_scale)*100
print(propVar_scale)
screeplot(pcaAnalysis_scale)
print(calcNoVars(propVar_scale))
```

##Answer: Fewer components are needed since outliers of the different parameters have a higher impact when they are not scaled accordingly. When scaled outliers have less impact and therefore the percentage of the variation for each component decreases.

##Write a code that fits a principle component regression ("utime" as response and all scaled numerical variables as features) with M components to the training data and estimates the training and test errors, do this for all feasible M values. Plot dependence of the training and test errors on M and explain this plot in terms of bias-variance tradeoff.

```
trainscore=c()
testscore=c()
library(pls)
pcamodel=pcr(utime~., 17, data=train, scale=TRUE)
for (i in 1:17) {
  pred_train=predict(pcamodel, ncomp=i)
  pred_test=predict(pcamodel, newdata=test, ncomp=i)
  trainscore[i]=mean((train$utime-pred_train)^2)
  testscore[i]=mean((test$utime-pred_test)^2)
}

plot(trainscore, xlab="Index", ylab="Error", col="blue", type="b", ylim=c(100,300))
points(testscore, xlab="Index", ylab="Error", col="red", type="b", ylim=c(100,300))
noOfPCA=which(testscore == min(testscore))
print(noOfPCA)
```

##Answer: When using more and more components the bias decreases and the variance goes up. The model performs better and better on training data. However, at one point the model becomes overfitted and performs worse on the test data as more components are added. The point where the model performs best on test data is when using 14 PCs.

##Use PCR model with M=8 and report a fitted probabilistic model that shows the connection between the target and the principal components.

```
pcamodel_new=pcr(utime~., 8, data=train, scale=TRUE)
pcamodel_new$Yloadings
mean(pcamodel_new$residuals^2)
```

##Answer: The formula is given by the loadings of the model and the variance is given by taking the average of the sum of squared residuals.

##Use original data to create variable “class” that shows “mpeg” if variable “codec” is equal to “mpeg4”, and “other” for all other values of “codec”. Create a plot of “duration” versus “frames” where cases are colored by “class”. Do you think that the classes are easily separable by a linear decision boundary?

```
Dataframe2=read.csv("video.csv")
Dataframe2=subset(Dataframe2, select=c(codec, frames, duration))
Dataframe2=cbind(Dataframe2, class=ifelse(Dataframe2$codec == 'mpeg4', 'mpeg', 'other'))
plot(Dataframe2$duration, Dataframe2$frames, col=c("red", "blue")[Dataframe2$class], xlab="Duration",
     ylab="Frames",
     main="Plot of duration vs frames")
```

##Answer: It seems that a linear decision boundary could separate the two classes rather well with exception of a few cases near the origin of the plot.

##Fit a Linear Discriminant Analysis model with “class” as target and “frames” and “duration” as features to the entire dataset (scale features first). Produce the plot showing the classified data and report the training error. Explain why LDA was unable to achieve perfect (or nearly perfect) classification in this case.

```
#Create function for misclassification rate
missclass=function(conf_matrix, fit_matrix){
  n=length(fit_matrix[,1])
  return(1-sum(diag(conf_matrix))/n)
}

library(MASS)
LDADData=Dataframe2
LDADData$duration=scale(LDADData$duration)
LDADData$frames=scale(LDADData$frames)
ldamodel=lda(class~duration+frames, data=LDADData)
predicted_lda=predict(ldamodel, data=LDADData)
confusion_matrix=table(LDADData$class, predicted_lda$class)
misclass=missclass(confusion_matrix, LDADData)
print(confusion_matrix)
print(misclass)
plot(Dataframe2$duration, Dataframe2$frames, col=c("red", "blue")[predicted_lda$class], xlab="Duration",
     ylab="Frames",
     main="Plot of duration vs frames after LDA")
```

##Answer: Because the two clusters of data don't have the same covariance matrix which can also be seen in the plot. The linear patterns are different for the two classes and have clearly different slopes.

##Fit a decision tree model with “class” as target and “frames” and “duration” as features to the entire dataset, choose an appropriate tree size by cross-validation. Report the training error. How many leaves are there in the final tree? Explain why such a complicated tree is needed to describe such a simple decision boundary.

```
library(tree)
treemodel=tree(class~duration+frames, data=Dataframe2)
summary(treemodel)
#Since number of terminal nodes is 11 we will check which number of leaves that is optimal in terms of lowest deviance
trainscore=rep(0,11)
for (i in 2:11) {
  prunedTree=prune.tree(treemodel, best=i)
  trainscore[i]=deviance(prunedTree)
}
plot(2:11, trainscore[2:11], type="b", col="red", ylim=c(0,700))
finalTree=prune.tree(treemodel, best=11)
temp=predict(treemodel, type="class")
confusion_matrix_tree=table(Dataframe2$class, temp)
tree_misclass= missclass(confusion_matrix_tree, Dataframe2)
print(confusion_matrix_tree)
print(tree_misclass)
```

##Answer: As seen in the plot the optimal number of leaves is the maximal one which is 11.

Assignment 2 – Neural networks

##Train a neural network (NN) to learn the trigonometric sine function. To do so, sample 50 points uniformly at random in the interval [0, 10]. Apply the sine function to each point. The resulting pairs are the data available to you. Use 25 of the 50 points for training and the rest for validation. The validation set is used for early stop of the gradient descent. Consider threshold values $i/1000$ with $i=1,...,10$. Initialize the weights of the neural network to random values in the interval [-1,1]. Consider two NN architectures: A single hidden layer of 10 units, and two hidden layers with 3 units each. Choose the most appropriate NN architecture and threshold value. Motivate your choice. Feel free to reuse the code of the corresponding lab.

Estimate the generalization error of the NN selected above (use any method of your choice).

In the light of the results above, would you say that the more layers the better ? Motivate your answer.

```
RNGversion('3.5.1')
#install.packages("neuralnet")
library(neuralnet)
set.seed(1234567890)
Var <- runif(50, 0, 10)
trva <- data.frame(Var, Sin=sin(Var))
train <- trva[1:25,] # Training
valid <- trva[26:50,] # Validation
n = dim(valid)[1]

# Random initialization of the weights in the interval [-1, 1] for model with 1 hidden layer
winit <- runif(31, -1, 1)
trainScore = rep(0,10)
validScore = rep(0,10)
for(i in 1:10) {
  nn_temp <- neuralnet(Sin~Var, data=train, hidden=10, threshold=i/1000, startweights=winit)
  nn = as.data.frame(nn_temp$net.result)
  pred=predict(nn_temp, newdata=valid)
  trainScore[i] = 1/n*sum((nn[,1]-train$Sin)^2)
```

```

  validScore[i] = 1/n*sum((pred-valid$Sin)^2)
}

#Random initialization of the weights in the interval [-1, 1] for model with two hidden layers
winit2=runif(22,-1,1)
trainScore2=rep(0,10)
validScore2=rep(0,10)
#R could not perform neuralnet analysis with thresholds smaller than 7/10. That is why the loop starts at 7.
for(i in 7:10) {
  nn_temp2 <- neuralnet(Sin~Var, data=train, hidden=c(3,3), threshold=i/1000, startweights=winit2)
  nn2 = as.data.frame(nn_temp2$net.result)
  pred2=predict(nn_temp2, newdata=valid)
  trainScore2[i] = 1/n*sum((nn2[,1]-train$Sin)^2)
  validScore2[i] = 1/n*sum((pred2-valid$Sin)^2)
}

plot(1:10, validScore[1:10], type="b", col="red", xlab="Threshold index", ylab="MSE")
plot(7:10, validScore2[7:10], type="b", col="blue", xlab="Threshold index", ylab="MSE")
min1=min(validScore[1:10])
min2=min(validScore2[7:10])
finalModel=ifelse(min1<min2, "1", "2")
optimal_i=ifelse(finalModel == '1', which(validScore[1:10] == min1, which(validScore2[7:10] == min2)))
print(finalModel)
print(optimal_i)

```

##Answer: The most appropriate model is using a one layer architecture with 10 units and using a threshold index of

##4/1000. This is because this model yields the lowest MSE when applied to the validation data.

#Generating new data for testing.

```

Var = runif(50, 0, 10)
test = data.frame(Var, Sin=sin(Var))
n=dim(test)[1]
winit = runif(31, -1, 1)
finalModel = neuralnet(Sin~Var, data=trva, hidden=10, threshold=4/1000, startweights=winit)
results=as.data.frame(finalModel$net.result)
pred = predict(finalModel, newdata = test)
genererror = 1/n*sum((pred-test$Sin)^2)
print(genererror)
plot(prediction(finalModel)$rep1)
points(test, col = "red")

```

2016-01-09

Assignment 1 – Tree, LASSO, Modified error function

##Dataset crx.csv contains encrypted information about the customers of a bank and whether each individual has paid back the loan or not: Class 1=paid back, 0=not paid back

##Divide the dataset into training and test sets (80/20), use seed 12345. Fit a decision tree with default settings to the training data and plot the resulting tree. Finally, remove the second observation from the training data, fit the tree model again and plot the tree. Compare the trees and comment why the tree structure changed so much although only one observation is deleted.

```

#Read data
RNGversion('3.5.1')
library(tree)

```

```

Dataframe=read.csv("crx.csv")
n=dim(Dataframe)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.8))
train=Dataframe[id,]
test=Dataframe[-id,]

treemodel=tree(Class~., data=train)
summary(treemodel)
plot(treemodel)
text(treemodel, pretty=0)
train_new=train[-2,]
treemodel_new=tree(Class~., data=train_new)
plot(treemodel_new)
text(treemodel_new, pretty=0)

```

##Answer: Tree structure does not change at all.

##Prune the tree fitted to the training data by using the cross-validation. Provide a cross-validation plot and comment how many leaves the optimal tree should have. Which variables were selected by the optimal tree?

```

cv.res=cv.tree(treemodel)
plot(cv.res$size, cv.res$dev, type="b", col="red")
plot(log(cv.res$k), cv.res$dev, type="b", col="red")
optimalTree=prune.tree(treemodel, best=3)
summary(optimalTree)
plot(optimalTree)
text(optimalTree, pretty=0)

```

##Answer: Two variables were selected for the optimal tree; A9 and A10. The best no of leaves is 3.

##Use this kind of code to prepare the feature set to be used with a LASSO model (here 'train' is the training data):

```

## x_train = model.matrix(~ .-1, train[,-16])
##Fit a LASSO model to the training data, carefully consider the choice of family parameter in the glmnet
function. Report the cross-validation plot, find the optimal penalty parameter value and report the number of
components selected by LASSO. By looking at the plot, comment whether the optimal model looks statistically
significantly better than the model with the smallest value of the penalty parameter.

```

```

x_train = model.matrix( ~ .-1, train[,-16])
library(glmnet)
class=as.factor(train$Class)
lassomodel=cv.glmnet(x_train, class, alpha=1, family="binomial")
lassomodel$lambda.min
plot(lassomodel)
coef(lassomodel, s="lambda.min")

```

##Answer: Optimal penalty parameter is 0.01036912 and the number of components used are 23. The optimal model does not look significantly better than when the smallest value is used.

##Use the following error function to compute the test error for the LASSO and tree models:

$E = \sum (Y_i * \log(\pi_i) + (1 - Y_i) * \log(1 - \pi_i))$ where Y_i is the target value and π_i are predicted probabilities of $Y_i=1$. Which model is the best according to this criterion? Why is this criterion sometimes more reasonable to use than the misclassification rate?

```

x_test = model.matrix( ~ .-1, test[,-16])
pred_lasso=predict(lassomodel, s=lassomodel$lambda.min, newx=x_test, type="response")

```

```
errorfunction=function(classvector, predvector) {
  return(sum(classvector*log(predvector)+(1-classvector)*log(1-predvector)))
}
```

```
pred_tree=predict(optimalTree, newdata=test, type="vector")
error_tree=errorfunction(test$Class, pred_tree)
error_lasso=errorfunction(test$Class, pred_lasso)
```

##The tree model is better according to this criterion. This criterion might be more suitable since it takes into account the probability of a class being classified and not just if it gets it right.

Assignment 2 – SVM with Kernel, nested cross-validation

##In the following steps, you are asked to use the R package kernlab to learn a SVM for classifying the spam dataset that is included with the package. For the C parameter consider values 1 and 5. Consider the radial basis function kernel (also known as Gaussian) and the linear kernel. For the former, consider a width of 0.01 and 0.05. This implies that you have to select among six models.

##Use nested cross-validation to estimate the error of the model selection task described above. Use two folds for inner and outer cross-validation. Note that you only have to implement the outer cross-validation: The inner cross-validation can be performed by using the argument cross=2 when calling the function ksvm. Hint: Recall that inner cross-validation estimates the error of the different models and selects the best, which is then evaluated by the outer cross-validation. So, the outer cross-validation evaluates the model selection performed by the inner cross-validation

```
RNGversion('3.5.1')
library(kernlab)
set.seed(12345)
data(spam)
n=dim(spam)[1]
id=sample(1:n, floor(n*0.5))
fold1=spam[id,]
fold2=spam[-id,]
C=c(5,1)
width=c(0.01,0.01,0.05,0.05,0,0)
kernel=c("rbfdot", "rbfdot", "rbfdot", "rbfdot", "vanilladot", "vanilladot")
```

```
missclass=function(conf_matrix, fit_matrix){
  n=length(fit_matrix[,1])
  return(1-sum(diag(conf_matrix))/n)
}
```

```
prediction=function(train, test, C, width, kernel) {
  if (width == 0) {
    svmmodel=ksvm(type~., data=train, kernel=kernel, C=C, cross=2)
  } else {
    svmmodel=ksvm(type~., data=train, kernel=kernel, C=C, cross=2, kpar=list(sigma=width))
  }
  predicted=predict(svmmodel, newdata=test)
  confusion=table(test$type, predicted)
  return(missclass(confusion, test))
}
```

```
scores=numeric(6)
scores2=numeric(6)
for (i in 1:6) {
```



```
scores[i]=prediction(fold1, fold2, C[(i %% 2)+1], width[i], kernel[i])
scores2[i]=prediction(fold2, fold1, C[(i %% 2)+1], width[i], kernel[i])
}
```

```
avgScore=(scores+scores2)/2
bestModel=which(avgScore == min(avgScore))
print(bestModel)
```

##Answer: Optimal model is using a C-value of 5, gaussian kernel with width 0.01.

##Produce the code to select the model that will be returned to the user.

#Final model

```
finalModel = ksvm(type~., data=spam, kernel="rbfdot", C=5, kpar=list(sigma=0.01), cross=2)
```

R

Examples

Linear regression

```
fit=lm(formula, data, subset, weights,...)
```

- data is the data frame containing the predictors and response values
- formula is expression for the model
- subset which observations to use (training data)?
- weights should weights be used?

fit is object of class lm containing various regression results.

- Useful functions (many are generic, used in many other models)
- Get details about the particular function by ".", for ex. predict.lm

```
summary(fit)
predict(fit, newdata, se.fit, interval)
coefficients(fit) # model coefficients
confint(fit, level=0.95) # CIs for model parameters
fitted(fit) # predicted values
residuals(fit) # residuals
```

Example of ordinary least squares regression

```
mydata=read.csv2("Bilexempel.csv")
fit1=lm(Price~Year, data=mydata)
summary(fit1)
fit2=lm(Price~Year+Mileage+Equipment, data=mydata)
summary(fit2)
```

Linear regression – confidence intervals

```
fitted <- predict(fit1, interval = "confidence")
# plot the data and the fitted line
attach(mydata)
plot(Year, Price)
lines(Year, fitted[, "fit"])
# plot the confidence bands
lines(Year, fitted[, "lwr"], lty = "dotted", col="blue")
lines(Year, fitted[, "upr"], lty = "dotted", col="blue")
detach(mydata)
```

Ridge regression

Use package glmnet with alpha = 0 (Ridge)

```
data=read.csv("machine.csv", header=F)
covariates=scale(data[,3:8])
response=scale(data[, 9])
model0=glmnet(as.matrix(covariates), response, alpha=0,family="gaussian")
plot(model0, xvar="lambda", label=TRUE)
```

Choosing best model using cross-validation

```
model=cv.glmnet(as.matrix(covariates), response, alpha=0,family="gaussian")
model$lambda.min
plot(model)
coef(model, s="lambda.min")
```

How good is this model in prediction?

```
ind=sample(209, floor(209*0.5))
data1=scale(data[,3:9])
train=data1[ind,]
test=data1[-ind,]
covariates=train[,1:6]
response=train[, 7]
model=cv.glmnet(as.matrix(covariates), response, alpha=1,family="gaussian", lambda=seq(0,1,0.001))
y=test[,7]
ynew=predict(model, newx=as.matrix(test[, 1:6]), type="response")
#Coefficient of determination
sum((ynew-mean(y))^2)/sum((y-mean(y))^2)
sum((ynew-y)^2)
```

Lasso regression

Use package glmnet with alpha = 1 (LASSO)

Stepwise selection (stepAIC, specify which way under *direction*)

```
library(MASS)
fit <- lm(V9~.,data=data.frame(data1))
step <- stepAIC(fit, direction="both")
step$anova
summary(step)
```

Holdout method (dividation into train, valid, test)

How to partition into train/test

```
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.7))
train=data[id,]
test=data[-id,]
```

How to partition into train/valid/test

```
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.4))
```

```

train=data[id,]
id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.3))
valid=data[id2,]
id3=setdiff(id1,id2)
test=data[id3,]

```

Cross-validation – K folds and different predictor sets

Try models with different predictor sets

```

data=read.csv("machine.csv", header=F)
library(cvTools)
fit1=lm(V9~V3+V4+V5+V6+V7+V8, data=data)
fit2=lm(V9~V3+V4+V5+V6+V7, data=data)
fit3=lm(V9~V3+V4+V5+V6, data=data)
f1=cvFit(fit1, y=data$V9, data=data,K=10, foldType="consecutive")
f2=cvFit(fit2, y=data$V9, data=data,K=10, foldType="consecutive")
f3=cvFit(fit3, y=data$V9, data=data,K=10, foldType="consecutive")
res=cvSelect(f1,f2,f3)
plot(res)

```

Logistic regression

Use `glm()` with family="binomial"

- Predicted probabilities: `predict(fit, newdata, type="response")`

Linear Discriminative Analysis (LDA) and Quadratic Discriminative Analysis (QDA)

Syntax in R: Library MASS

`lda(formula, data, ..., subset, na.action)`

- Prior – class probabilities
- Subset – indices, if training data should be used

`qda(formula, data, ..., subset, na.action)`

`predict(..)`

Naïve bayes

Use package e1071

```

library(MASS)
library(e1071)
n=dim(housing)[1]
ind=rep(1:n, housing[,5])
housing1=housing[ind,-5]
fit=naiveBayes(Sat~., data=housing1)
fitYfit=predict(fit, newdata=housing1)
table(Yfit,housing1$Sat)

```

Decision trees

Use package *tree*, alternative *rpart*

```

tree(formula, data, weights, control, split = c("deviance", "gini"), ...)
print(), summary(), plot(), text()

```

Example

```
library(tree)
n=dim(biopsy)[1]
fit=tree(class~., data=biopsy)
plot(fit)
text(fit, pretty=0)
fit
summary(fit)
```

Misclassification results

```
Yfit=predict(fit, newdata=biopsy, type="class")
table(biopsy$class,Yfit)
```

Selecting optimal tree by penalizing

- Use Cv.Tree()

```
set.seed(12345)
ind=sample(1:n, floor(0.5*n))
train=biopsy[ind,]
valid=biopsy[-ind,]
fit=tree(class~.,data=train)
set.seed(12345)
cv.res=cv.tree(fit)
plot(cv.res$size, cv.res$dev, type="b", col="red")
plot(log(cv.res$k), cv.res$dev, type="b", col="red")
```

Selecting optimal tree by train/validation

```
fit=tree(class~., data=train)
trainScore=rep(0,9)
testScore=rep(0,9)
for(i in 2:9) {
  prunedTree=prune.tree(fit,best=i)
  pred=predict(prunedTree, newdata=valid, type="tree")
  trainScore[i]=deviance(prunedTree)
  testScore[i]=deviance(pred)
}
plot(2:9, trainScore[2:9], type="b", col="red", ylim=c(0,250))
points(2:9, testScore[2:9], type="b", col="blue")
```

Use final tree decided by methods above

```
finalTree=prune.tree(fit, best=5)
Yfit=predict(finalTree, newdata=valid, type="class")
table(valid$class,Yfit)
```

Least Absolute Deviation (LAD) regression

Use package L1pack

Bootstrap

Use package boot

Functions:

- Boot()
- Boot.ci() – 1 parameter

- Envelope() – many parameters

Example: `boot(data, statistic, R, sim="ordinary", ran.gen = function(d, p) d, mle=NULL, ...)`

Random random generation for parametric bootstrap:

- `Rnorm()`
- `Runif()`
- ...

Nonparametric bootstrap:

- Write a function statistic that depends on dataframe and index and returns the estimator

```
library(boot)
data2=data[order(data$a$Area),]#reordering data according to Area
# computing bootstrap samples
f=function(data, ind){
  data1=data[ind,]# extract bootstrap sample
  res=lm(Price~Area, data=data1) #fit linear model
  #predict values for all Area values from the original data
  priceP=predict(res,newdata=data2)
  return(priceP)
}
res=boot(data2, f, R=1000) #make bootstrap
```

Parametric bootstrap

- Compute value mle that estimates model parameters from the data
- Write function `ran.gen` that depends on data and mle and which generates new data
- Write function statistics that depend on data which will be generated by `ran.gen` and should return the estimator

```
mle=lm(Price~Area, data=data2)
summaryMLE = summary(mle)
rng=function(data, mle ) {
  data1=data.frame(Price=data$Price, Area=data$Area)
  n=length(data$Price)
  #generate new Price
  data1$Price=rnorm(n,predict(mle, newdata=data1),sd(summaryMLE$residuals))
  return(data1)
}
```

```
f1=function(data1){
  res=lm(Price~Area, data=data1) #fit linear model
  #predict values for all Area values from the original data
  priceP=predict(res,newdata=data2)
  return(priceP)
}
res=boot(data2, statistic=f1, R=1000, mle =mle, ran.gen=rng , sim="parametric")
```

Bootstrap confidence bands for linear model

```
e=envelope(res) #compute confidence bands
fit=lm(Price~Area, data=data2)
priceP=predict(fit)
plot(Area, Price, pch=21, bg="orange")
points(data2$Area,priceP,type="l") #plot fitted line
#plot confidence bands
```

```
points(data2$Area,e$point[2,], type="l", col="blue")
points(data2$Area,e$point[1,], type="l", col="blue")
```

Bootstrap prediction bands for linear model

```
mle=lm(Price~Area, data=data2)
f1=function(data1){
  res=lm(Price~Area, data=data1) #fit linearmodel
  #predictvaluesfor all Area valuesfrom the original data
  priceP=predict(res,newdata=data2)
  n=length(data2$Price)
  predictedP=rnorm(n,priceP, sd(mle$residuals))
  return(predictedP)
}
res=boot(data2, statistic=f1, R=10000, mle=mle, ran.gen=rng, sim="parametric")
```

Principle Component Analysis (PCA)

- Formulas: `Prcomp()`, `biplot()`, `screeplot()`
- Use package `pls` for making Principle component regression

```
mydata=read.csv2("tecator.csv")
data1=mydata
data1$Fat=c()
res=prcomp(data1)
lambda=res$sdev^2
#eigenvalues
lambda
#proportion of variation
sprintf("%2.3f",lambda/sum(lambda)*100)
screeplot(res)
```

Principal component loadings (U)

```
U=res$rotation
head(U)
```

Data in (PC1, PC2) – scores (Z)

```
plot(res$x[,1], res$x[,2], ylim=c(-5,15))
```

Trace plots

```
U= res$rotation
plot(U[,1], main="Traceplot, PC1")
plot(U[,2],main="Traceplot, PC2")
```

Probabilistic PCA

- Use `pcaMethods` from Bioconductor

Independent Component Analysis (ICA)

R package: `fastICA`

```
S <- cbind(sin((1:1000)/20), rep((((1:200)-100)/100), 5))
A <- matrix(c(0.291, 0.6557, -0.5439, 0.5572), 2, 2)
X <- S %*% A #mixing signals
```

```
a <- fastICA(X, 2) #now separate them
```

Distance between geographical points of interest

Use package geosphere

Use function distHaversine(x, y) which returns the distance between the two points whereas x and y are 2 dimensional vectors/data frames (i.e. pairs of coordinates of latitude and longitude)

Neural networks

Use package neuralnet

Use function neuralnet(formula, data, hidden, threshold, startweights)

- Formula – $X \sim Y$
- Data – the data used
- Hidden – the number of nodes in each hidden layers (can be vector of c(5, 3) which corresponds to first hidden layer with 5 nodes and second hidden layer with 3 nodes)
- Threshold – the threshold of the partial derivatives of the error function as stopping criteria
- Startweights – a vector containing starting values of the weights (needs to be initialized), if NULL random initialization