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Labs

Lab 1

Assignment 1 – Logistic regression and KKNN-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 Y(hat) = 1 if p(Y=1 | X) > 0.5, otherwise Y(ha
t)=0 and report the confusion matrices (use table()) and the misclassification rat
es 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 missclassification 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 com
pared to the test data. However, the fact that the miscalculations are similar ind
icates that the model performs similarly on two different data sets which is gener
ally 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 princi
ple: 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
```

```r
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 mod
el is well fitted, since the model acts similar between trained and tested data. A
lthough this classificiation principle gives us a higher misclassification rate, i
t 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 misclas
sification 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 set
s differ alot. This shows us that our model is not well fitted. The misclassificat
ion is lower for the trained data, since the model is fitted after these values. C
ompared to the results from using logistic regression to classify the data, the re
sults from the KKNN model were significally worse on the test data. This implies t
hat KKNN 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. U
sing 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*e^(-theta*x) for x = Length in whi
ch observations are independent and identically distributed. What is the distribut
ion type of x. Write a function that computes the log-likelihood log p(x|theta) fo
r a given theta and a given data vector x. Plot the curve showing the dependence o
f log-likelihood on theta where the entire data is used for fitting. What is the m
aximum likelihood value of theta 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(Datafram
e), 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 t
ype exponential. The maximum
##likelihood value of theta is: 42.29453 The optimal theta 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 m
aximum 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="r
ed", ylim=c(0,100))
curve(-loglikelihood(x, y), xlab="Theta", from=0, to=20, add=TRUE, col="blue", yli
m=c(0,100))

#Conclusion: The graph is increasing at a much slower pace when only using the fir
st 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 wher
```

```
eas the one with only six values, the theta value could be anything from the minim
um value and forward.

#4: Assume now a Bayesian model with p(x|theta)=theta*e^(-theta*x) and a prior p(t
heta)=lambda*e^(-lambda*x), lambda=10
#Write a function computing l(theta)=log(p(x|theta)*p(theta)). What kind of measur
e is actually computed by this
#function? Plot the curve showing the dependence of l(theta) on theta computed usi
ng the entire data and overlay it with a plot from step 2. Find an optimal theta a
nd 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, t
o=10, add=TRUE, col="blue",
      ylim=c(20,300))

#Conclusion: When using an bayesian model we have a prior that gives the model inf
ormation beforehand which helps
#fitting the model. The optimal theta is now 0.91 which is close to the datasets m
eanvalue, 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|thet
a)=theta*e^(-theta*x) (use standard number generators). Create the histograms of t
he 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 betwee
n the actual and predicted data. This concludes model was accurately fitted to the
 correct distribution model.
```

```r
#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 appropri
ate

#2: Consider model Mi 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. M1 is a linear m
odel, M2 is a quadratic model and so on). Report a probabilistic model that descri
bes Mi. Why is it appropriate to use MSE criterion when fitting this model to a tr
aining data?

#Conclusion: A probabilistic model describing M(i) is: M(i) = w0 + w1 * X + w2 * X
2 + ... + wi * Xi (3) The MSE
#criterion is a suitable method since it punishes outliers to a larger extent. Thi
s creates a better fitted model
#compared to when you punish the absolute value. This reduces the risk of an overf
itted model.

#3: Divide the data into training and validation sets (50%/50%) and fit models Mi,
 i=1,...,6.  For each model, record the training and the validation MSE and presen
t 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 orig
```

```r
inal 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 t
est 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 t
he lowest MSE and therefore being the model with the smallest error. In terms of b
ias, what we can see is that in the training model the predicted error, and MSE, i
s 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 teste
d data and the MSE decreases for the training data. Variance is defined by the dif
ference 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 c
hosen 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 th
e 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)

#Conclusion: 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 l
arge values more).

#7: Choose the best model by cross validation for LASSO model. Report optimal lamb
da and how many variables that
#chosen by the model and make conclusions. Present also a plot showing the depende
nce 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 increas
e. 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 where 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", su
b="Red = Female, Blue = Male",
     col=c("red", "blue")[Dataframe$sex], xlab="CL", ylab="RW")

#Create function for misclassification rate
```

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

#Conclusion: Yes the classification seems to be linearly separable. However, the t
wo clusters of data clearly have different covariance matrices (since angle of tre
nd is different) which is not optimal for the LDA method.

#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 misclassi
fication 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")

#Conclusion: When comparing the graph from step 1 and the graph of the predicted v
alues it is noteable that the
#classifications do not differ that much. With a misclassification rate of only 0.
035 and 200 datapoints it can be concluded that 7 observations were classified inc
orrectly. When comparing the graphs it is difficult to find the points which have
changed color (since they have been classified incorrectly) but one example is the
 point farthest to the let which was classified as male but should have been class
ified as female. The model classifies the data accurately.

#3: Repeat step 2 but use priors p(Male)=0.9 and p(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(Male)=0.9 and
p(Female)=0.1"
     , sub="Red = Female, Blue = Male", col=c("red", "blue")[predicted2$class], xl
ab="CL", ylab="RW")

#Conclusion: From this graph we can see that a few more data points were classifie
d incorrectly. This is due to the higher prior set on classifying a data point as
male, i.e. 0.9. It is noteable in the confusion matrix that no males classified in
correctly. This is also due to the high prior which basically says that is is not
that likely that a datapoint will be classified as a female. When the model in fac
t classify a data point as female it has to be sure of it, and this can be seen as
 stated above in the confusion matrix. On the other hand, more females are classif
ied as males inaccurately since the higher prior. This also results in a higher mi
sclassification rate of 0.08.

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

```
he 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), y
lim=c(0,20))

boundaryline = function(length, coefficientvector, prior) {
  return(-coefficientvector[1]/coefficientvector[3]-(coefficientvector[2]/coeffici
entvector[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")

#Conclusion: When using logistic regression the results are similar as the first b
uilt model with LDA. This is simply a coincident and no real conclusion can be dra
wn regarding the exact same misclassification rate except from that the models see
m to classify the data in a similar way. When comparing which data points that are
 classified as females and males in the two models it can be concluded that the mo
del using logistic regression classifies the data in a way which enables a boundar
y line more distinctly. This is due to the characteristics of the logistic regress
ion model. The equation for the decision boundary line is as follows: RW(hat)=-(be
ta0+beta1*CL)beta2
```

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,]
```

```r
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 devi
ance. 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

#Conclusion: It can be concluded from the misclassification rates that the split m
ethod deviance, classifies the data in a better way than the split method gini. Si
nce the method deviance performed better it will be the chosen splitting method in
 the following steps.

#3: Use training and valid data to choose optimal tree depth. Present graphs of th
e 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 te
st 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)
```

```r
#Final tree contains variables savings, duration and history. Since 3 vars => Dept
h 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)

#Conclusion: The tree with the lowest deviance used 4 leaves which is the optimal
tree. The variables used by the tree is savings, duration and history, and the dep
th of the tree is 3. The misclassification rate for the test data is 0.256.

#4: Use traning data to perform classification using Naives bayes and report the c
onfusion matrices and
#misclassification rates for the traning and for the test data. Compare with resul
ts from previous steps.

#Load libraries
library(MASS)
library(e1071)
fit_naive=naiveBayes(good_bad~., data=train)
#Create function for predicting and creating confusion matrice and printing miscla
ssification 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)

#Conclusion: With the naive bayes method the misclassification rate is higher than
 what was concluded in step 3.
#The misclassification rate for test data for the naive bayes method is 0.316 and
the misclassification rate for the decision tree from step 3 is 0.256. This indica
tes that the decision tree method classifies the data more accurately than what th
e model which uses the naive bayes method does.

#5: Use optimal tree and Naives Bayes to classify the test data by using principl
e: 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 corresponsing 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)
```

```r
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

#Conclusion: From the ROC-curve we cam see that the total area under the curve (AO
C) is the biggest for the naive
#bayes method. Therefore this method should be the one to use instead of the decis
ion tree model.

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

naiveModel=naiveBayes(good_bad~., data=train)
```

```r
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, "go
od", "bad"))
misclass_testLoss=misclass(confusion_testLoss, test)
print(confusion_testLoss)
print(misclass_testLoss)

#Conclusion: 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 3 – Bootstrap with tree models

```r
#1: Reorder your data with respect to the increase of MET and plot EX versus MET.
Discuss what kind of model can be appropriate here. Use the reordered data in step
s 2-5.

RNGversion('3.5.1')
#Read data
set.seed(12345)
Dataframe=read.csv2("State.csv")
Dataframe=Dataframe[order(Dataframe$MET),]
MET=Dataframe$MET
EX=Dataframe$EX

plot(MET, EX, xlab="EX", ylab="MET", type="p", main="Plot of EX vs MET")

#Conclusion: Some kind of squared model might be useful here.

#2: Use package tree  and fit a regression tree model with target EX and feature M
ET in which the number of the leaves is selected by cross-validation, use the enti
re data set and set minimum number of observations in a leaf equal to 8 (setting m
incut in tree.control).  Report the selected tree. Plot the original and the fitte
d data and histogram of residuals. Comment on the distribution of the residuals an
d the quality of the fit.

library(tree)
treemodel=tree(EX~MET, data=Dataframe, control=tree.control(48, mincut=8))
summary(treemodel)
plot(treemodel)
text(treemodel, pretty=0)
set.seed(12345)
cvTreeModel = cv.tree(treemodel)
plot(cvTreeModel$size, cvTreeModel$dev, type="b", col="red", xlab="Size", ylab="De
v")
bestSize = cvTreeModel$size[which.min(cvTreeModel$dev)]
bestTree=prune.tree(treemodel, best=bestSize)
plot(bestTree)
text(bestTree, pretty=0)
title("Optimal tree")
```

```r
predData=predict(bestTree, newdata=Dataframe)
plot(MET, EX, xlab="EX", ylab="MET", type="p", col="red", main="Plot original vs p
redicted data")
points(MET, predData, col="blue")
summaryfit=summary(bestTree)
hist(summaryfit$residuals, breaks=10)

#Conclusion: The distribution of the residuals seems to be fairly normally distrib
uted with no bias. The fit is quite good considering the simple model that it is.

library(boot)
# computingbootstrapsamples
f=function(data, ind){
  data1=data[ind,]# extractbootstrapsample
  treeModel=tree(EX~MET, data=data1, control=tree.control(48, mincut=8))
  prunedtree=prune.tree(treeModel, best=3)
  predData=predict(prunedtree,newdata=Dataframe)
  return(predData)
}
res=boot(Dataframe, f, R=1000) #make bootstrap
confIntNPBoot=envelope(res)
plot(MET, EX, xlab="EX", ylab="MET", pch=21, bg="orange", main="Plot original vs p
redicted data", ylim=c(100,500))
points(MET, predData, type="l", col="blue")
points(MET, confIntNPBoot$point[2,], type="l")
points(MET, confIntNPBoot$point[1,], type="l")

#Conclusion: The confidence bands are bumpy. This is due to the fact that no distr
ibution is assumed for the data. The model will try to accostom as best it can fro
m the data given. The width of the confidence band is rather high which indicates
that the model used is not that reliable. Furthermore we can almost draw a straigh
t line between the whole band which would mean that each EX value would yield the
same MET value which again implies that the model is not that good.

mle=prune.tree(treemodel, best=3)
summaryMLE = summary(mle)
rng=function(data, mle) {
  data1=data.frame(EX=data$EX, MET=data$MET)
  n=length(data$EX)
  #generatenew EX
  data1$EX=rnorm(n,predict(mle, newdata=data1), sd(summaryMLE$residuals))
  return(data1)
}

f1=function(data1){
  treemodel=tree(EX~MET, data=data1, control=tree.control(48,mincut=8)) #fit linea
rmodel
  prunedtree=prune.tree(treemodel, best=3)
  n=length(Dataframe$EX)
  #predictvaluesfor all EX values from the original data
  predData=predict(prunedtree,newdata=Dataframe)
  predictedEX=rnorm(n, predData, sd(summaryMLE$residuals))
  return(predictedEX)
}
res=boot(Dataframe, statistic=f1, R=1000, mle=mle, ran.gen=rng, sim="parametric")
predIntPBoot=envelope(res)
points(MET, predIntPBoot$point[2,], type="l", col="green")
points(MET, predIntPBoot$point[1,], type="l", col="green")
```

```
#Conclusion: NOTE: This code above is wrong. The confidence bands for parametric b
ootstrap shold be computed separately The confidence bands retrieved are more smoo
th. However when looking at the residuals they do not seem to be normally distribu
ted as assumed. Therefore a parametric bootstrap model is not preffered => choose
non-parametric.
```

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

```
#1: 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", ma
in="PC1 vs PC2", xlab="PC1",
     ylab="PC2")
#We can see from the graph that the data is very accurately described by PC1.

#Conclusion: From the screeplot it can be conlcuded that the two components captur
es almost all of the variation in the data. Therefore PCA analysis is suitable for
 the data. Two components capture 99.5957 % of the variation and therefore these t
wo components will be used in the following steps. Most of the data points are aro
und 0 for PC1 but there are some data points which can be described as outliers lo
cated to the farthest right in the score plot.

#2: Make trace plots of the loadings of the components selected in step 1. Is ther
e any principle component that is explaines 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")

#Conclusion: We can see from graph that PC2 is not described by so many original f
eatures since it is close to zero for many of the features. The last 30 or so vari
ables 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 fo
llowing:
# Compute W'=K*W and present columns of W' in form of the trace plots. Compare wit
h 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 t
he 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")
plot(icaModel$S[,1], icaModel$S[,2], main="ICA1 vs ICA2", xlab="ICA1", ylab="ICA2
", type="p", col="blue")

#Conclusion: When comparing the trace plots of ICA1 and ICA2 with PC1 and PC2 from
 step 2, it is noteable that for the first component the dependency on the feature
s increases as the index increases. It is also noteable that the plots for the dif
ferent components appear to be each others mirrors. This is reasonable because PCA
 tries to maximize the variance, i.e. look for correlation between the different f
eatures, whereas ICA tries to do the exact opposite, i.e. maximizing the independe
nce between the different features by creating an orthogonal coordinate system. Th
e parameter W' which is computed by W(hat)=K*W describes how the features explain
the principal components ICA1 and ICA2. When comparing the last score plot with th
e score plot from step 1 it can also be concluded that the score plot of ICA is mi
rroring the score plot of PCA. However, the axis of the coordinate system of ICA h
ave been standardized wh  ich is the difference between the plots.
```

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 pla
ce 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 i
n 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 measureme
nt
##    was made and the day of interest.
```

```r
##  The third to account for the distance between the hour of the day a temperatur
e measurement
##    was made and the hour of interest.
## Choose an appropriate smoothing coefficient or width for each of the three kern
els above.
## Answer to the following questions:
##  Show that your choice for the kernels' width is sensible, i.e. that it gives m
ore weight
##    to closer points. Discuss why your of definition of closeness is reasonable.
##  Instead of combining the three kernels into one by summing them up, multiply t
hem.
##    Compare the results obtained in both cases and elaborate on why they may dif
fer.
## Note that the file temps50k.csv may contain temperature measurements that are p
osterior
## 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 t
he 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 bir
th 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="Da
ys")
```

```r
}

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="Hou
rs")
}

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=" "), forma
t="%Y-%m-%d %H:%M:%S"),
                        strptime(paste(data$date, data$time, sep=" "),format="%Y-%m
-%d %H:%M:%S")))>0), ])
}

#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 ker
nel 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", xl
ab="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))

#Conclusion: When studying the graphs above further, the h values can be motivate
d. Finally, the estimations for the temperatures are made through the summation of
 different kernel functions as well as multiplication of the different Kernel func
tions. The summation of kernel functions provides estimates closer to the mean of
all temperatures (4.62) than what the multiplication of kernel functions has provi
ded. This can be due to that data points which have received a high weight through
 the kernel functions will have more impact in the multiplication of kernel functi
ons than with the summation of kernel functions, and similarily data points which
have received a low weight through the kernel functions will have more impact in t
he multiplication of kernel functions than with the summation of kernel functions.
 To conclude, the three different weights in the multiplication of kernel function
s all has to be quite high in order for the total weight to be high. On the other
hand if one weight is low the whole weight is going to be low even though the othe
r two are high. The result of this is that the data points with high weight is mor
e significant and perhaps more similar to the point of interest and time of intere
st for the multiplication of kernels than for the summation of kernels. This can a
lso be seen in the graphs where the temperatures for the multiplication of kernels
 seem more reasonable intuitively than for the summation of kernels and seem like
a more accurate model.
```

Assignment 2 – Support vector machines

```
##Use the function ksvm from the R package kernlab to learn a SVM for classifying
the spam dataset that is included with the package. Consider the radial basis func
tion kernel (also known as Gaussian) with a width of 0.05. For the parameter C, co
```

```
nsider values 0.5, 1 and 5. This implies that you have to consider three models.
# Perform model selection, i.e. select the most promising of the three models (use
 any method of your choice except cross-validation or nested-cross-validation)
# Estimate the generalization error of the SVM selected above (use any method of y
our choice except cross-validation or nested cross validation)
# Produce the SVM that will be returned to the user, i.e. show the code
# What is the purpose of the parameter C?

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)

##Conclusion: 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 e
mails, 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(sigm
a=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.

#Final model

finalmodel=ksvm(type~., data=spam, kernel="rbfdot", kpar=list(sigma=0.05), C=1)
```

Assignment 3 – Neural networks, weight initialization

```
## Assignment3:
## Train a neural network to learn the trigonometric sine function. To do so, samp
le 50 points
## uniformly at random in the interval [0,10]. Apply the sine function to each poi
nt. The resulting
## pairs are the data available to you. Use 25 of the 50 points for training and t
he 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 ar
e below a given
## threshold value. Check the argument threshold in the documentation.Consider thr
eshold
## values i/1000 with i = 1,...,10. Initialize the weights of the neural network t
o random values in
## the interval [-1, 1].  Use a neural network with a single hidden layer of 10 un
its. 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 w
ith 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, startweig
hts=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="MS
E")
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)
```

```
##Conclusion: As seen in the graph, naturally the train data performs the best whe
n the threshold value is as small as possible, i.e. 1/1000, and the performance de
creases as this threshold increases for the train data. From the graph we can see
that the threshold value 4/1000 performs the best on the validation data (since it
 results in the lowest MSE) and therefore this threshold will be used moving forwa
rd in the assignment.

optimal_nn = neuralnet(Sin~Var, data=train, hidden=10, threshold=optimal_i/1000, s
tartweights=winit)
plot(optimal_nn)
# Plot of the predictions (black dots) and the data (red dots)
plot(prediction(optimal_nn)$rep1)
points(trva, col = "red")

##Conclusion: The optimal neural network with threshold 4/1000 is chosen which res
ults in the neural network shown above. The last two graphs briefly show how simil
ar the predicted values from the model are in comparison to the real sinus curve.
One can conclude that the neural network created resembles the shape of the sinus
curve with quite a precision.
```

Exam

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 p
aid back

##Divide the dataset into training and test sets (80/20), use seed 12345. Fit a de
cision tree with default settings to the training data and plot the resulting tre
e. Finally, remove the second observation from the training data, fit the tree mod
el again and plot the tree. Compare the trees and comment why the tree structure c
hanged 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. Provid
e a cross-validation plot and comment how many leaves the optimal tree should hav
```

```
e. 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 n
o 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 optim
al penalty parameter value and report the number of components selected by LASSO.
By looking at the plot, comment whether the optimal model looks statistically sign
ificantly 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 use
d are 23. The optimal model does not look significantly better than when the small
est value is used.

##Use the following error function to compute the test error for the LASSO and tre
e models:
##E=sum(Yi*log(pi)+(1-Yi)*log(1-pi)) where Yi is the target value and pi are predi
cted probabilities pf Yi=1. Which model is the best according to this criterion? W
hy is this criterion sometimes more reasonable to use than the misclassification r
ate?

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

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 mo
re suitable since it takes into account the probability of a class being classifie
d 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 SV
M for classifying the spam dataset that is included with the package. For the C pa
rameter consider values 1 and 5. Consider the radial basis function kernel (also k
nown 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 de
scribed above. Use two folds for inner and outer cross-validation. Note that you o
nly have to implement the outer cross-validation: The inner cross-validation can b
e performed by using the argument cross=2 when calling the function ksvm. Hint: Re
call that inner cross-validation estimates the error of the different models and s
elects the best, which is then evaluated by the outer cross-validation. So, the ou
ter cross-validation evaluates the model selection performed by the inner cross-va
lidation

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)
```

2017-04-18

Assignment 1 – Naïve bayes, logistic regression, PCA

```
##Plot the dependence of CW versus BD where the points are colored by Species. Are
 CW and BD good predictors of the Species?

#Read data
RNGversion('3.5.1')
Dataframe=read.csv("australian-crabs.csv")
CW=Dataframe$CW
BD=Dataframe$BD
plot(CW, BD, col=c("blue", "orange")[Dataframe$species], main="Plot of CW vs BD",
sub="Blue = blue, Orange=orange")

##Answer: It seems like they are since it is a clear distinction between the two c
lusters of data. A linear predictor seems like a good way of classifying the data.

##Create a Naïve Bayes classifier model with Species as target and CW and BD as pr
edictors. Present the confusion matrix and comment on the quality of the classific
ation. Based on the assumptions of the Naïve Bayes, explain why this model is not
appropriate for these data

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


library(MASS)
library(e1071)
fit_naive=naiveBayes(species~CW+BD, data=Dataframe)
pred=predict(fit_naive, newdata=Dataframe, type="class")
confusion_naive=table(Dataframe$species, pred)
print(confusion_naive)
misclass_naive=misclass(confusion_naive, Dataframe)

##Answer: The quality of the fit seems to be rather bad since the model misclassif
ies 39,5 % of the data according to the misclassification rate. Since the data is
strongly correlated and the method of using Naive bayes implies an assumption of i
ndependent features it is reasonable that the model does not perform that well, ag
ain since it is clear from the plot that the two features used, CW and BD are stro
ngly correlated.

##Fit the logistic regression now with Species as target and CW and BD as predicto
rs and present the equation of the decision boundary. Plot the classified data and
 the decision boundary and comment on the quality of the classification

glmmodel=glm(species~CW+BD, data=Dataframe, family="binomial")
pred_glm=predict(glmmodel, newdata=Dataframe, type='response')
species_vector=as.factor(c(ifelse(pred_glm>0.5, 'Orange', 'Blue')))
confusion_glm=table(Dataframe$species, species=ifelse(pred_glm>0.5, 'Orange', 'Blu
e'))
```

```
print(confusion_glm)
plot(CW, BD, main="Plot predicted values of CW and BD but with logistic regression
",
     col=c("blue", "orange")[species_vector], xlab="CW", ylab="BD", xlim=c(18,53),
 ylim=c(5,22),
     sub="Red = Female, Blue = Male, Green = Boundaryline")

boundaryline = function(length, coefficientvector, prior) {
  return(-coefficientvector[1]/coefficientvector[3]-(coefficientvector[2]/coeffici
entvector[3])*length+
           log(prior/(1-prior))/coefficientvector[3])
}

curve(boundaryline(x, glmmodel$coefficients, 0.5), col="green", add=TRUE)
glmmodel$coefficients

##Answer: The quality of the classification is as expected really good (since look
ing at the plot, a linear classifier seemed appropriate). The model only misclassi
fied 4 points which yielded a low misclassification rate. The equation for the bou
ndary line is as follows: BD=-0.484810/9.432817+CW*3.624760/9.432817

##Scale variables CW and BD and perform principal component analysis with these tw
o variables. Present the proportion of variation explained by PC1 and PC2 and base
d on results from step 1 explain why the first principal component contains so muc
h variation. Present the equations expressing principal component coordinates thro
ugh the original coordinates.

pcaData=Dataframe[,7:8]
pcaData=scale(pcaData)
response=as.vector(Dataframe$species)
pcaAnalysis=prcomp(pcaData)
lambda=pcaAnalysis$sdev^2
#Eigenvalues
print(lambda)
#Proportion of variation
propVar= lambda/sum(lambda)*100
screeplot(pcaAnalysis)
print(propVar)
summary(pcaAnalysis)
X=pcaData
coeff=pcaAnalysis$rotation
Z=X%*%coeff

##Answer: Since we could se a clear pattern in the plot from step 1, PCA analysis
will select the angle of the line as its first principle component since across th
is line we can find the most variation in the data. Since the data was so strongly
 correlated, almost all of the variation in the data can be explained by just one
 PCA component. The equation expressing principle component coordinates through th
e original ones is as follows: PCACoordinates=X*coefficientsMatrix, i.e. PCACoordi
nates=X*pcaAnalysis$rotation.
##Equations separately: PC1=CW*0.7071068+BD*0.7071068, PC2=CW*(-0.7071068)+BD*0.70
71068

##Create a Naïve Bayes classifier model with Species as target and PC1 and PC2 as
predictors. Compute the confusion matrix and explain how much the classification q
uality has changed and why.

naiveData=as.data.frame(cbind(pcaAnalysis$x, species=response))
naiveModelPCA=naiveBayes(species~PC1+PC2, data=naiveData)
```

```r
predPCA=predict(naiveModelPCA, newdata=naiveData, type="class")
confusion_naivePCA=table(Dataframe$species, predPCA)
print(confusion_naivePCA)
misclass_naivePCA=misclass(confusion_naivePCA, Dataframe)

##Answer: The classification is now 100 % correct. This is due to the fact that th
e two PCA components derived are mutually independent of each other which makes na
ive bayes classifier a perfect fit since this is exactly what the model is assumin
g.
```

Assignment 2 – Poisson distributed linear model, bootstrap prediction band

```r
##File bank.csv shows the number of customers (Visits) that arrived to a bank duri
ng various time slots (Time) between 9.00 and 12.00.

##Fit a generalized linear model in which response is Poisson distributed, and the
 canonical link (log) is used for regression. Report the probabilistic expression
for the fitted model (how the target is distributed based on the feature)

#Read data
RNGversion('3.5.1')
Dataframe=read.csv2("bank.csv")

linear_model=glm(Visitors~., data=Dataframe, family="poisson")
linear_model$coefficients
control=exp(0.1742155+0.4017126*seq(9,12,0.1))
print(control)

##Answer: The probabilistic expression for the target is Visitors=e^(0.1742155+0.4
017126*Time). The control vector shows that the response variable resulted from th
e equation is fairly reasonable and resembles the original data.

##Compute a prediction band for the values of Time=12,12.05,12.1,…,13.0 by using t
he model from step 1 and the parametric bootstrap with B=1000. Plot the original d
ata values and the prediction band into one figure and comment whether the band se
ems to give a correct forecasting. How many customers (report a range) should the
bank expect at 13.00?

library(boot)
rng=function(data, mle) {
  data1=data.frame(Visitors=data$Visitors, Time=data$Time)
  n=length(data$Visitors)
  #generate new Price
  data1$Visitors=rnorm(n,predict(mle, newdata=data1), sd(mle$residuals))
  return(data1)
}

f1=function(data1){
  res=lm(Visitors~., data=data1) #fit linearmodel
  #predictvaluesfor all Visitor valuesfrom the original data
  Visitors=predict(res,newdata=data.frame(Time=seq(12,13,0.05)))
  n=length(seq(12,13,0.05))
  predictedVisitors=rnorm(n, Visitors, sd(linear_model$residuals))
  return(predictedVisitors)
}
res=boot(Dataframe, statistic=f1, R=1000, mle=linear_model, ran.gen=rng, sim="para
metric")
e=envelope(res)
plot(Dataframe$Time, Dataframe$Visitors, main="Forecasting of visitors depending o
n time", xlab="Time",
```

```
     ylab="Visitors", xlim=c(9,13), ylim=c(30,500))
points(seq(12,13,0.05), exp(e$point[2,]), type="l", lty=21, col="gray")
points(seq(12,13,0.05), exp(e$point[1,]), type="l", lty=21, col="gray")

min_value_13=exp(e$point[2,21])
max_value_13=exp(e$point[1,21])
cat("The bank should expect between", min_value_13, "and", max_value_13, "customer
s", sep=" ")

##Answer: The band seems to give a correct forecasting. The bank should expect bet
ween approx 177 and 281
##customers at 13:00.
```

2018-01-11

Assignment 1 – PCA, PCA regression, LDA, tree

```
#Read data and divide randomely 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 sc
aling 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 h
ave a higher impact when they are not scaled accordingly. When scaled outliers hav
e less impact and therefore the percentage of the variation for each component dec
```

```
reases.

##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 dat
a and estimates the training and test errors, do this for all feasible M values. P
lot 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(100,30
0))
points(testscore, xlab="Index", ylab="Error", col="red", type="b", ylim=c(100,30
0))
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 betterand better on training data. However, at one poi
nt the model becomes overfitted and performs worse on the test data as more compon
ents are added. The point where the model performs best on test data is when using
 14 PC:s.

##Use PCR model with M=8 and report a fitted probabilistic model that shows the co
nnection 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 gi
ven by taking the average of the sum of squared residuals.

##Use original data to create variable "class" that shows "mpeg" if variable "code
c" 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 th
at 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$codec == 'mpeg4', 'mpeg', 'ot
her'))
plot(Dataframe2$duration, Dataframe2$frames, col=c("red", "blue")[Dataframe2$clas
s], 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 d
ata 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)
LDAData=Dataframe2
LDAData$duration=scale(LDAData$duration)
LDAData$frames=scale(LDAData$frames)
ldamodel=lda(class~duration+frames, data=LDAData)
predicted_lda=predict(ldamodel, data=LDAData)
confusion_matrix=table(LDAData$class, predicted_lda$class)
misclass=missclass(confusion_matrix, LDAData)
print(confusion_matrix)
print(misclass)
plot(Dataframe2$duration, Dataframe$frames, col=c("red", "blue")[predicted_lda$cla
ss], 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 w
hich can also be seen in the plot. The linear patterns are different for the two c
lasses 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 i
s 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 whic
h is 11.
```

Assignment 2 – Neural networks, difference between layers

```
##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 funct
```

```r
ion to each point. The resulting pairs are the data available to you. Use 25 of th
e 50 points for training and the rest for validation. The validation set is used f
or 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 int
erval [-1,1]. Consider two NN architectures: A single hidden layer of 10 units, an
d two  hidden layers with 3 units each. Choose the most appropriate NN architectur
e and threshold value. Motivate your choice. Feel free to reuse the code of the co
rresponding lab.
##Estimate the generalization error of the NN selected above (use any method of yo
ur 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 hi
dden 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, startweig
hts=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 h
idden 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, star
tweights=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="MS
E")
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])
```

```r
finalModel=ifelse(min1<min2, "1", "2")
optimal_i=ifelse(finalModel == '1', which(validScore[1:10] == min1, which(validSco
re2[7:10] == min2)))
print(finalModel)
print(optimal_i)

##Answer: The most appropriate model is using a one layer architecture with 10 uni
ts and using a threshold index of 4/1000. This is because this model yields the lo
west MSE when applied to the validation data. No, it is not always best to use mul
tiple layers as seen in this example.

#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, startweigh
ts=winit)
results=as.data.frame(finalModel$net.result)
pred = predict(finalModel, newdata = test)
generror = 1/n*sum((pred-test$Sin)^2)
print(generror)
plot(prediction(finalModel)$rep1)
points(test, col = "red")
```

2019-01-16

Assignment 1 – Poisson distributed maxlikelihood, Poisson LASSO regression, tree, PCA

```r
##The data file Influenza.csv contains contains the number of registered cases of
influenza and mortality.

##Assume that mortality y is poisson distributed. Write an R code computing the mi
nus-loglikelihood of Mortality values for a given λλ (use only basic R functions,
do not use implemented Poisson distribution in R). Compute the minus log-likelihoo
d values for  λλ = 10,110,210, … , 2910 and produce a plot showing the dependence
of the minus log-likelihood on the value of λλ. Define the optimal value of λλ by
means of visual inspection (i.e. approximately).

RNGversion('3.5.1')

Dataframe=read.csv("Influenza.csv")
Mortality=Dataframe$Mortality

like=function(y, lambda){
  n=length(y)
  return(lambda*n-log(lambda)*sum(y)+sum(log(factorial(y))))
}

#Find maximum likelihood value of theta
lambda_max = function(y){
  n=length(y)
  return(sum(y)/n)
}

lambda_max=lambda_max(Mortality)
lambda=seq(10,2910,100)
plot(like(Mortality, lambda), lambda, main="The minus loglike function of mortalit
y depending on Lambda",
```

```
     xlim=c(10,2910))

##Answer: Towards infinity, don't know how to fix

##Scale all variables except of Mortality. Divide the data randomly (50/50) into t
raining and test sets and fit a LASSO regression with Mortality as a Poisson distr
ibuted target and all other variables as features. Select the optimal parameters i
n the LASSO regression by the crossvalidation and report the optimal LASSO penaliz
ation parameter and also the test MSE. Is the MSE actually the best way of measuri
ng the error rate in this case? Report also the optimal LASSO coefficients and rep
ort which variables seem to have the biggest impact on the target. Check the value
 of intercept αα, compute exp(αα) and compare it with the optimal λλ in step 1. Ar
e these quantities similar and should they be?

library(cvTools)
library(glmnet)

features=scale(Dataframe[,-3])
data=cbind(features, Mortality)

n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]
test=data[-id,]
covariates=train[,1:8]
response=train[,9]

lassomodel=cv.glmnet(as.matrix(covariates), response, alpha=1, family="poisson")
opt_lambda=lassomodel$lambda.min
plot(lassomodel)
coef(lassomodel, s="lambda.min")
y=test[,9]
ynew=predict(lassomodel, newx=as.matrix(test[,1:8]), type="response", s="lambda.mi
n")
MSE=mean((ynew-y)^2)
interceptval=exp(coef(lassomodel, s="lambda.min")[1])

##Answer: Optimal lasso coefficients shown above. The feature year is not used. Th
e features Influenza,
##temperature.deficit and influenza_lag2 seem to have the biggest impact on the ta
rget. The exponential of the
##intercept alpha is similar to the optimal lambda in step 1. This is due to the f
act that the link between a poisson distribution and the calculated mean is the lo
g-function. By applying exp to the intercept we thereby receive a value which corr
esponds to the calculated mean of lambda.

##Fit a regression tree with Mortality as a target and all variables as a features
 and select the optimal size of the tree by cross-validation. Report the test MSE
and compare it with the MSE of the LASSO regression in step 2. Why is it not reaso
nable to do variable selection by applying LASSO penalization also to the tree mod
els?

library(tree)
train=as.data.frame(train)
test=as.data.frame(test)
treemodel=tree(Mortality~., data=train)
set.seed(12345)
cv.res=cv.tree(treemodel)
```

```r
plot(cv.res$size, cv.res$dev, type="b", col="red")
bestSize=cv.res$size[which(min(cv.res$dev) == cv.res$dev)]
finalTree=prune.tree(treemodel, best=bestSize)
plot(finalTree)
text(finalTree, pretty=0)
yFit=predict(finalTree, newdata=test, type="vector")
MSE_tree=mean((yFit-test$Mortality)^2)

##Answer: The MSE for the tree model is higher than for the LASSO-model which impl
ies that the LASSO model should be used since it performs better. It is not reason
able to do LASSO penalization to tree model because the tree model is not continuo
us but discrete.

##Perform principal component analysis using all the variables in the training dat
a except of Mortality and report how many principal components are needed to captu
re more than 90% of the variation in the data. Use the coordinates of the data in
the principal component space as features and fit a LASSO regression with Mortalit
y as a Poisson distributed target by crossvalidation, check penalty factors λλ =
0, 0.1, 0.2, … , 50. Provide a plot that shows the dependence of the cross-validat
ion error on log(λλ). Does complexity of the model increase when λλ increases? How
 many features are selected by the LASSO regression? Report a probabilistic model
corresponding to the optimal LASSO model.

PCAdata=subset(train, select=-Mortality)
pcaAnalysis=prcomp(PCAdata, scale=FALSE)
screeplot(pcaAnalysis)
lambda=pcaAnalysis$sdev^2
print(lambda)
#Proportion of variation
propVar=lambda/sum(lambda)*100
print(propVar)
#Function for calculating the number of components needed for explaining at least
95% of the variation.
calcNoVars = function(data){
  noOfVars=1
  sumOfVariation=data[noOfVars]
  while(sumOfVariation<90){
    noOfVars=noOfVars+1
    sumOfVariation=sumOfVariation+data[noOfVars]
  }
  return(noOfVars)
}
print(calcNoVars(propVar))
summary(pcaAnalysis)
new_base=pcaAnalysis$x
set.seed(12345)
lasso_PCA=cv.glmnet(new_base[,1:5], response, alpha=1, family="poisson", lambda=se
q(0,50,0.1))
plot(lasso_PCA)
opt_lambda_PCA=lasso_PCA$lambda.min
coef(lasso_PCA, s="lambda.min")

##Answer: 5 components are needed to describe more than 90 % of the variation in t
he data. The complexity of the model decreases as lambda increases since a higher
lambda penalizes the coefiicients more. 3 features are selected by the LASSO regre
ssion. The probabilistic model is: Yi~P(exp(7.484554465-0.035756922*PC1-0.00939520
5*PC2-0.004745676*PC3+0.011627449*PC4+0.003882809*PC5))
```

Assignment 2 – Neural networks, converge against value, analyze weights, SVMs

```
##You are asked to use the function neuralnet of the R package of the same name to
 train a neural network (NN) to
##mimic the trigonometric sine function. You should run the following code to obta
in the training and test data.

##Produce the code to train the NN on the training data tr and test it on the data
 te. Use a single hidden layer with three units. Initialize the weights at random
in the interval [-1,1]. Use the default values for the rest of parameters in the f
unction neuralnet. You may need to use the function compute. Confirm that you get
results similar to the following figure. The black dots are the training data. The
 blue dots are the test data. The red dots are the NN predictions for the test dat
a.

library(neuralnet)
set.seed(1234567890)
Var <- runif(50, 0, 3)
tr <- data.frame(Var, Sin=sin(Var))
Var <- runif(50, 3, 9)
te <- data.frame(Var, Sin=sin(Var))
n = dim(tr)[1]
# Random initialization of the weights in the interval [-1, 1]
winit <- runif(10, -1, 1)
nn=neuralnet(Sin~Var, data=tr, hidden=3, startweights=winit)
pred=predict(nn, newdata=te)
plot(tr$Var, tr$Sin, xlim=c(0,9), ylim=c(-2,2), xlab="Var", ylab="Sin")
points(te$Var, te$Sin, col="blue")
points(te$Var, pred, col="red")

##Answer: The plot resembles the one given so it is confirmed.

##In the previous figure, it is not surprising the poor performance on the range
[3,9] because no training point falls in that interval. However, it seems that the
 predictions converge to -2 as the value of Var increases. Why do they converge to
 that particular value ? To answer this question, you may want to look into the we
ights of the NN learned.

sigmoid=function(input){
  return(1/(1+exp(-input)))
}

z1=sigmoid(0.61705*te$Var-1.51988)
z2=sigmoid(1.995*te$Var-1.27708)
z3=sigmoid(-1.61733*te$Var+4.89639)
y=-3.92871*z1+2.67522*z2+0.84607*z3-0.62953
print(y)

##Answer: When Var goes towards infinity the first and second node in the hidden l
ayer is activated and the third
##node in the hidden layer is not. This yields an approximate response value of -
3.92871+2.67522-0.62953 (bias)=-1,88302 which can be seen in the graph.

##You are asked to use the function ksvm from the R package kernlab to learn a sup
port vector machine (SVM) to classify the spam dataset that is included with the p
ackage. You should use the radial basis function kernel (also known as Gaussian) w
ith a width of 0.05.
# You should select the most appropriate value for the C parameter, i.e. you shoul
d perform model selection. For this task, you can use any method that you deem app
ropriate.
```

```r
# In the previous question, you may have obtained an error message “no support vectors found” for C = 0. Can you give a plausible explanation for this error ?
# Estimate the generalization error of the SVM with the C value selected above. Use any method of your choice.
# Once a SVM has been fitted, a new point is essentially classified according to the sign of a linear combination of support vectors. You are asked to produce the pseudocode (no implementation is required) for computing this linear combination. Your pseudocode should make use of the functions alphaindex, coef and b. See the help of ksvm for information about these functions.

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],]

C=seq(0.2,10.2,0.5)
trainScore=numeric(21)
validScore=numeric(21)
for(i in 1:length(C)){
  svmmodel=ksvm(type~., data=train, kernel="rbfdot", kpar=list(sigma=0.05), C=C
[i])
  pred=predict(svmmodel, newdata=valid)
  confusion=table(valid$type, pred)
  validScore[i]=missclass(confusion, valid)
}
plot(1:21, validScore, col="red", type="b")
bestModel=which(min(validScore) == validScore)
bestParam=C[bestModel]

finalModel=ksvm(type~., data=spam[index[1:3501],], kernel="rbfdot", kpar=list(sigm
a=0.05), C=bestParam)
finalPred=predict(svmmodel, newdata=test)
finalConfusion=table(test$type, finalPred)
finalMisclass=missclass(finalConfusion, test)

##Answer: The optimal C-value is 1.2. When C=0 and no support vector was found you
 still are under the assumption that the data is linearly separable. When no suppo
rt vector is found I assume that the data is not linearly separable. The generaliz
ation error for the optimal model is approximately 0.08.
```

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 – classprobabiliies
•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(dat a$Area),]#reorderingdata accordingto Area
# computingbootstrapsamples
f=function(data, ind){
data1=data[ind,]# extractbootstrapsample
res=lm(Price~Area, data=data1) #fit linearmodel
#predictvaluesfor all Area valuesfrom 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$Price)
#generatenew Price
data1$Price=rnorm(n,predict(mle, newdata=data1),sd(summaryMLE$residuals))
return(data1)
}

f1=function(data1){
res=lm(Price~Area, data=data1) #fit linearmodel
#predictvaluesfor all Area valuesfrom 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) #computeconfidencebands
fit=lm(Price~Area, data=data2)
priceP=predict(fit)
plot(Area, Price, pch=21, bg="orange")
points(data2$Area,priceP,type="l") #plotfittedline
#plotcofidencebands
points(data2$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
- $rotation – the coefficients

```
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~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

Additional functions

Distributions

- Normal distribution (gaussian, link="identity")
  - `dnorm(x, mean = 0, sd = 1, log = FALSE)`
  - `pnorm(q, mean = 0, sd = 1, lower.tail = TRUE, log.p = FALSE)`
  - `qnorm(p, mean = 0, sd = 1, lower.tail = TRUE, log.p = FALSE)`
  - `rnorm(n, mean = 0, sd = 1)`
- Exponential distribution
  - `dexp(x, rate = 1, log = FALSE)`
  - `pexp(q, rate = 1, lower.tail = TRUE, log.p = FALSE)`
  - `qexp(p, rate = 1, lower.tail = TRUE, log.p = FALSE)`
  - `rexp(n, rate = 1)`
- Poisson distribution (link = log)
  - `dpois(x, lambda, log = FALSE)`
  - `ppois(q, lambda, lower.tail = TRUE, log.p = FALSE)`
  - `qpois(p, lambda, lower.tail = TRUE, log.p = FALSE)`
  - `rpois(n, lambda)`
- Binomial distribution (link = logit)
  - `dbinom(x, size, prob, log = FALSE)`
  - `pbinom(q, size, prob, lower.tail = TRUE, log.p = FALSE)`
  - `qbinom(p, size, prob, lower.tail = TRUE, log.p = FALSE)`
  - `rbinom(n, size, prob)`

Useful functions

- sapply(x, y) – input x in specified function y, returns vector of response values.
- Strptime(x, format="%Y-%m-%d %H:%M:%S") – convert string to datetime object with specified format
- Format(date, format="%H") – returns the specified part of the format string of a datetime object
- Cbind(x, y) – adds culumns y to x
- Rbind(x, y) – adds rows y to x
- Ifelse(eval, true, false) – returns true if eval is TRUE and false otherwise
- Which(x) – returns the TRUE indices of the eval x
- Optimize(function, interval) – optimizes the function specified over the interval specified
- Lty in plot – specifies sign of symbols (21 for confidence intervals)
- Nrow(Dataframe) – number of rows in dataframe
- Ncols(Dataframe) – number of columns in dataframe
- Paste(x, y, sep="") – join multiple vectors together
- Data(x) – load a built-in dataset into the environment
- X[c(1, 5)] – selects elements 1 and 5
- Is-na(a) – is missing
- Is.null(a) – is null
- L[[2]] – second element of list
- L[1] – new list with only first element
- L$x – element named x
- L['y'] – new list with only element named y

Ggplot

Ggplot(data, aes(x=x,y=y, colour=class)) +
Geom_point()

Standard home-made functions

Misclassification rate

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

Boundary line for logistic regression

```
boundaryline = function(length, coefficientvector, prior) {
  return(-coefficientvector[1]/coefficientvector[3]-
(coefficientvector[2]/coefficientvector[3])*length+
           log(prior/(1-prior))/coefficientvector[3])
}
```

Compare test and train scores for pruned tree

```
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)
}
```

Classify data in to class according to prior

```
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)
}
```

Calc TPR and FPR to use in ROC-curve

```
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)
}
```

Estimate error for different neural network models

```
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)
}
```

Theory

- General error estimation – trained data tested on not before seen test data. Often train model on train data, optimize parameters on validation data. Train chosen model on train and validation data and test generalization error on test data
- Model returned to user – the model which is trained on all the data available. Estimated data is the generalization error
- Naïve bayes – assumption: strong independence between variables. When applying PCA system with naïve bayes you receive very good classifiers since all the features in PCA are independent of each other.

Degrees of freedom

- Larger covariance => larger connection => better approximation => model more complex

Ridge regression

- High degree of polynomial leads to overfitting
- Theorem MAP estimate to the Bayesian ridge is equal to solution in frequentist ridge
- Particularly useful if the explanatory variables are strongly correlated to each other
- Degrees of freedom decrease when lambda increases

LASSO regression

- Yields sparse solution due to square compared to ridge which is circle

Bias-variance trade-off

- If bias(y(hat)(x0))=0, the estimator is unbiased

- ML estimators are asymptotically unbiased if the model is enough complex
- However, unbiasedness does not mean a good choice
- Risk = actual variance + bias ^2 + var(estimator)
- When model complexity increases, bias goes down and variance goes up and vice versa
-

Logistic regression

- Proof

$$\log\left(\frac{p(y=1|x,w)}{p(y=0|x,w)}\right) = \log\left(\frac{\frac{1}{1+e^{-w^T x}}}{1-\frac{1}{1+e^{-w^T x}}}\right) = \log\left(\frac{1}{1+e^{-w^T x}} * \frac{1+e^{-w^T x}}{e^{-w^T x}}\right) = w^T x$$

$$logit(t) = \log\frac{t}{1-t}$$

$$softmax(z) = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

Linear discriminative analysis

- Use log(ratio) for the boundary line to be linear
- Important: covariance matrices are the same
- Difference between logistic regression:
    - Coefficients estimated differently
- Not robust to outliers
- LDA is often a good classifier even if the assumption of normality and common covariance matrix are not satisfied

Naïve bayes

- Special case of LDA with diagonal covariance matrix – assumes mutual independence between features
- MLE are means and variances (per class)

Trees

- Regression trees
    - Target is a continuous variable
- Classification trees
    - Target is a class (qualitative) variable
- Number of areas in graph represent the number of leaves and terminal nodes of tree
- Normal model leads to regression trees
    - Objective: MSE to evaluate
- Mulitnoulli model leads to classification trees
    - Objective: cross-entropy (deviance)
- Robust to outliers
- High variance: small change in response => totally different tree
- Lack of smoothness
- Large trees may be needed to model an easy system

Models

- Normally distributed targets => linear regression
- Bernoulli and multinomial targets => logistic regression

Link functions

- F is link function (in principle arbitrary)
- F^-1 is activation function

Args against deterministic models

- The model does not really describe actual data (error is not explained)
    - No difference in modelling data A (Poisson) and B (Normal)
    - Estimation strategy for A is not good for B
- The model typically gives a deterministic answer, no information about uncertainty

Bootstrap

- Nonparametric bootstrap can be applied to any deterministic estimator, distribution-free
- Parametric bootstrap is however more exact if the distribution form is correct
- Bootstrap works for all distribution types
- Can be bad for small datasets, for example when n<40
- Parametric bootstrap works even for small samples

PCA

- Data become more approximate (but less data to store)
- PC1, … , PCM are eigenvectors of sample covariance
- Another view: minimize the distance between the original and projected data
- Do we need to scale features?
    - If scaling, less likely to have same direction as original base
    - You need to scale data
    - Don't want to scale data if all components is in same scale (e.g. in centimeters or meters)
    - Otherwise, <u>always</u> scale
- Equation: new base Z=X*Um where X is original data and Um is the coefficients (e.g. $rotation)
- Approx X values: X(approx.) = Z*Um(transpose) where columns have been removed to only use most important PCA components in Z

ICA

- Probabilistic PCA does not capture latent factors
    - Rotation invariance
- ICA assumes latent features are independent
    - Assuming noise-free x
- Convert X into PCA coordinate system: X'=XU
- Z=X'V
- Full transformation matrix: Uica=U*V

Kernel

Gaussian kernel: $k(u) = \exp(-||u||2)$ where $||\cdot||$ is the Euclidean norm.

- Cauchy kernel: $k(u) = 1/(1 + ||u||D+1)$
- Epanechnikov kernel: $k(u) = (1 - ||u||2)1_{\{||u||\leq 1\}}$
- Moving window kernel: $k(u) = 1_{\{u\in S(0,1)\}}$

- Small width implies considering few points. So, the variance will be large (similar to variance of a single point). The bias will be small since the points considered are close to x.
- Large width implies considering many points. So, the variance will be small and the bias will be large
- Cross-validation (K-fold): Not always best to choose large K (big train set) since this implies large variance on the test set (since it is so small), K=5, 10 works well

Support vector machines

- With no penalty, assumes that training set is linearly separable in the feature space (but not necessarily in input space)
- Aim for the separating hyperplane that maximizes the margin (i.e. the smallest perpendicular distance from any point to the hyperplane) so as to minimize the generalization error
- When adding penalty for penalizing misclassified points we drop assumption of linear separability in feature space

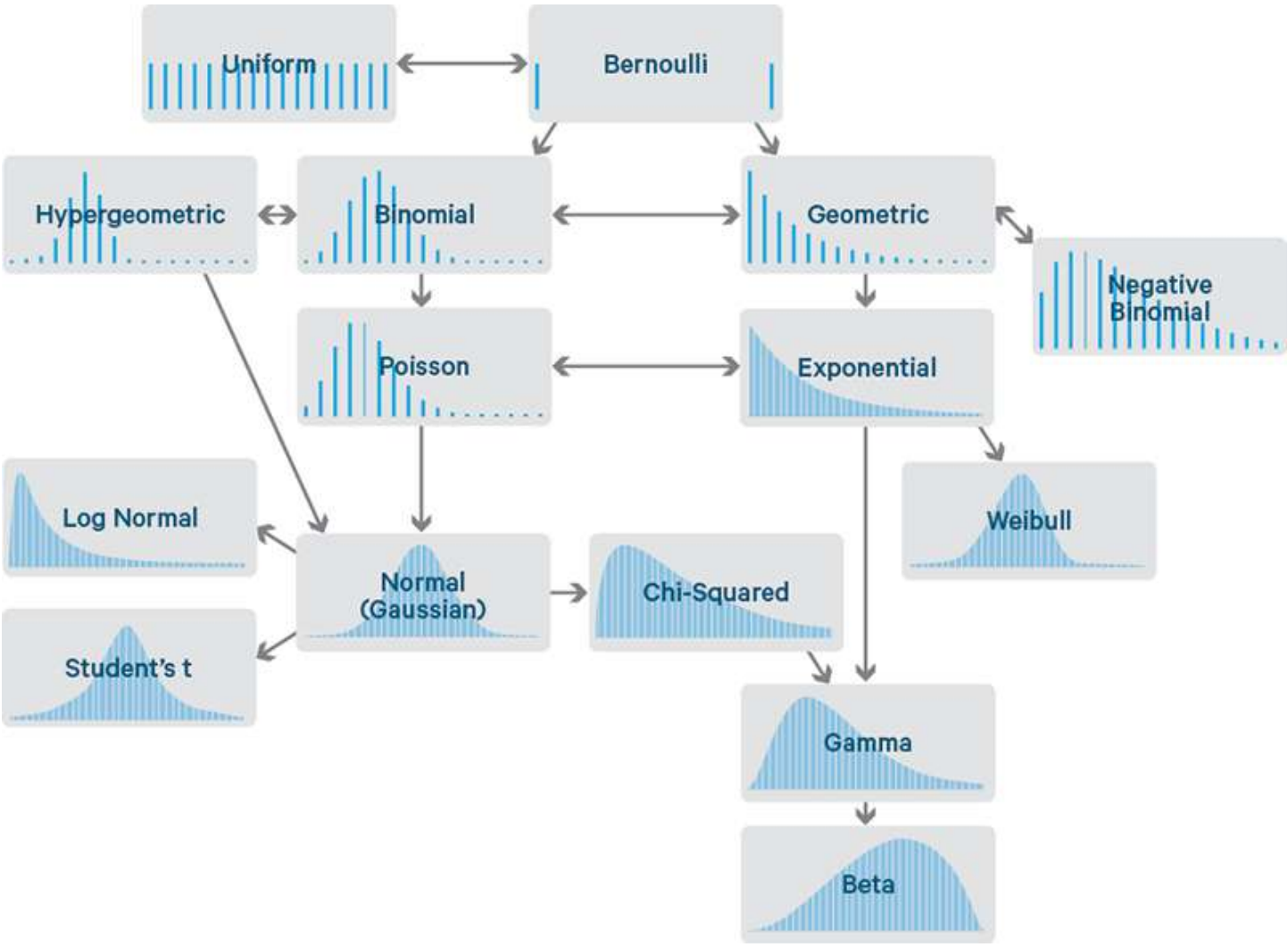
- A higher C implies penalizing violation of constraints more which yields a more non-smooth support vector. Creation of “islands” around points for example to avoid misclassification

Neural networks

- SVMs imply data-selected user-defined basis functions
- NNs imply a user-defined number of data-selected basis functions
- Neural networks is the same as ordinary linear classifiers without its activation functions
- For a large variety of activation functions, the two-layer NN can uniformly approximate any continuous function to arbitrary accuracy provided enough hidden units
- Initialize weights at random, but
    - Too small magnitude values may cause losing signal in the forward or backward passes, and
    - Too big magnitude values may cause the activation function to saturate and lose gradient
- Initialize the weights according to prior knowledge: Almost-zero for hidden units that are unlikely to interact, and bigger magnitude for the rest
- Initialize the weights to almost-zero values so that the initial model is almost-linear, i.e. sigmoid functions is almost linear around the zero. Let the algorithm to introduce non-linearities when needed
    - Note however that this initialization makes the sigmoid function take a value around half its saturation level. That is why hyperbolic tangent function (tanh(x)) is sometimes preferred in practise

Lecture notes

Probability density functions for common distributions



Kom ihåg newdata vs data Krav för LDA: data ska vara normalfördelad i varje klass och ha samma varians i båda klasserna. (Multivariate normality) Linear Discriminant Analysis. Dock kan LDA vara en bra metod för at classificera.

För att göra tree:s så behöver man göra om target till factors om den är non numeric. Använd: as.factor

När man gör general error estimation (out of sample error) så använder man både validation och training data och sen testar på test-data

"Model to give to the user" : train on all data (train + valid + test), estimated error is the generalization error

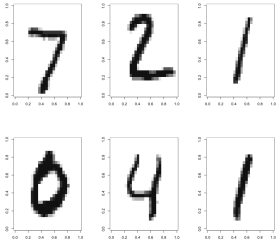
Knn.cv för crossvalidationi knn, library

Assumption Naive Bayes: You assume strong independence of the features

Logistic regression: glm(formula , data=data, family = "binomial")

Link funktioner (canonical link): logit :ln(p/(1-p) eller som in r log(p/(1-p) Log: ln(p) eller log(p)

Example: classifying hadwritten digits



Example: classifying hadwritten digits

Training data: 60000 images.
Test data: 10000 images.
Features: intensities (0-255, scaled to 0-1) in the $28 \times 28 = 784$ pixels as features.

Methods:
- Multinomial regression with LASSO prior
- Support vector machines
- Neural Networks (deep?)

Example: classifying hadwritten digits

- Confusion matrix

PREDICTION / TRUTH

	0	1	2	3	4	5	6	7	8	9
0	966	0	8	1	1	7	9	2	4	6
1	0	1121	1	1	0	2	3	13	7	7
2	2	2	957	13	5	4	4	21	7	0
3	0	2	9	947	0	29	1	3	12	10
4	0	0	12	1	940	5	5	9	8	32
5	6	1	3	19	1	816	9	1	24	9
6	4	4	13	1	7	12	926	0	10	1
7	1	0	9	10	2	2	0	954	5	13
8	1	4	17	11	2	10	1	3	892	4
9	0	1	3	6	24	5	0	22	5	927

Example: smartfone typing predictions

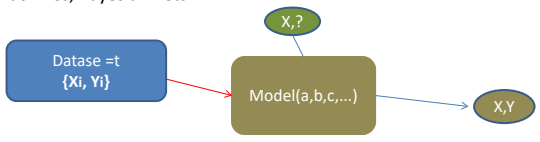
Example: smartfone typing predictions

- Assume a simple (Markov) model of a sentence:
$$p(w_1, \dots, w_n) = p(w_1)p(w_2|w_1) \dots p(w_n|w_{n-1})$$
- Intuition:
  - $p(person|crazy) = 0.1$
  - $p(horse|crazy) = 0.0001$

  Highest P(?|Donald) ?
- Probability for sentence depends only on $p(w_n|w_{n-1})$
- How to compute ? Investigate a lot of data!
$$p(w_k|w_{k-1}) = \frac{\#\ cases\ w_k\ follows\ w_{k-1}}{\#\ cases\ w_k}$$
- In practice, more advanced model used
  - Neural networks for ex.

Types of learning

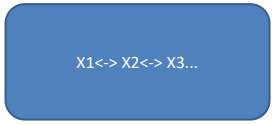
- **Supervised learning** (classification, regression)
  - Compute parameters from data
  - Given features of a new object, predict target
  - **Classification** (Y=categorical), **Regression** (Y=continuous)
- Most of ML models: Neural Nets, Decision Trees, Support Vector Machines, Bayesian nets



Types of learning

- Unsupervised learning (→Data Mining)
  - No target
  - Aim is to extract interesting information about
    - Relations of parameters to each other
    - Grouping of objects

Ex: clustering, density estimation, association analysis



Types of learning

- **Semi-supervised**: targets are known only for some observations.
- **Active learning**. Strategies for deciding which observations to label
- **Reinforcement learning**. Find suitable actions to maximize the reward. True targets are discovered by trial and error.

Basic ML ingridients

- **Data** D: observations (cases)
  - Features $X_1, \dots X_p$
  - Targets $Y_1, \dots, Y_r$

Case	X_1	X_2	Y
1			
2			
...			

- **Model** $P(x|\ w_1, \dots w_k)$ or $P(y|x, w_1, \dots w_k)$
  - Example: Linear regression $p(y|x, w) = N(w_0 + w_1 x, \sigma^2)$
- **Learning procedure** (data→get parameters $\hat{w}$ or $p(w|D)$)
  - Maximum likelihood, Bayesian estimation…
- **Prediction** of new data X^{new} by using the fitted model

Types of data sets

- **Training data** (training set D): used for fitting the model
  - Supervised learning: w_i in $P(y|\boldsymbol{x}, w_1, \dots w_k)$ estimated using D

X	Y
1.1	M
2.3	F

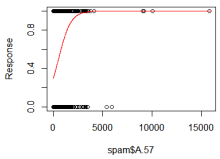
- **Test data** (test set T): used for predictions
  - Supervised learning: estimate $p(Y)$ or $\hat{Y}$ for new $\boldsymbol{x}$

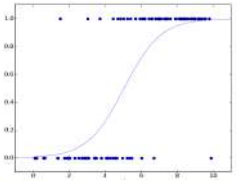
X	Y
1.3	?
2.9	?

Logistic regression

- Data $Y_i \in \{Spam, Not\ Spam\}, X_i = \#of\ a\ word$
- Model: $p(Y = Spam|w, x) = \frac{1}{1+e^{-w_0-w_1 X}}$
- Fitting: maximum likelihood
- Prediction : $p(spam) = p(Y = spam|x)$

We can also make point predictions -how?

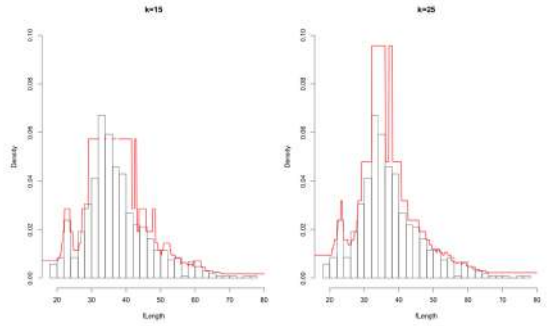




K-nearest neighbor density estimation

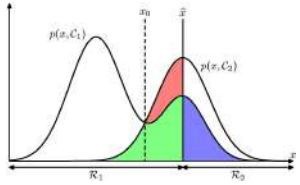
- Data: Fish length $X_1, \dots X_N$
- Model $p(x|K) = \frac{K}{N \cdot \Delta}$
  - K: #neighbors in training data
  - Δ: length of the interval containing K neighbors
- Learning: Fix some K or find an appropriate K
- Prediction: predict $p(x|K)$

K-nearest neighbor density estimation



K-nearest neighbor density estimation

- Why estimating a density can be interesting:
  1. Estimate **class-conditional densities** $p(x|y = C_i)$
  2. Predict

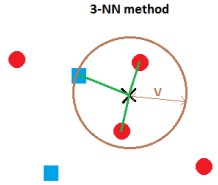


K-nearest neighbor classification

- Given N observations $(\boldsymbol{X}_j, Y_j)$
  - $Y_j = C_i$, where $C_1, \dots C_m$ are possible class values
- Model assumptions
  - Apply K-NN density estimation:

$$p(X = x|Y = C_i) = \frac{K_i}{N_i V}, p(C_i) = \frac{N_i}{N}$$

  - V: volume of the sphere
  - K_i: #obs from training data of $Y = C_i$ in the sphere
  - N_i: #obs from training data of $Y = C_i$



Bayesian classification

- Prediction $\hat{Y}(\boldsymbol{x}) = C_l$

$$l = \arg \max_{i \in \{1,\dots,m\}} p(C_i|\boldsymbol{x})$$

- Bayes theorem

$$p(C_i|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|C_i)p(C_i)}{p(\boldsymbol{x})}$$

- We get

$$p(C_i|x) \propto \frac{K_i}{K}$$

K-nearest neighbor classification

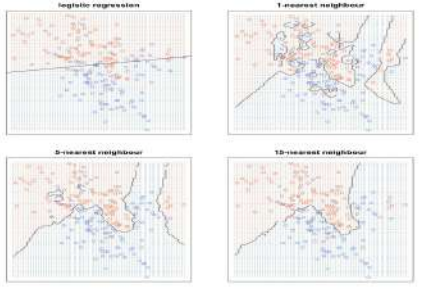
Algorithm

1. Given training set D,number K, and test set T
2. For each $x \in T$
   1. For each $i = 1, \dots M$
      1. $p'(C_i|x) = \frac{K_i}{K}$
   2. Compute $l = \arg \max_{i \in \{1,\dots,m\}} p'(C_i|\boldsymbol{x})$
   3. Predict $\hat{Y}(x) = C_l$

Majority voting: prediction for x is defined by majority voting of K neighbors

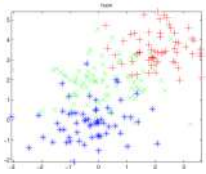
K-nearest neigbor example

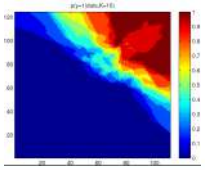
Why classification results are so different for K-NN?



Model types

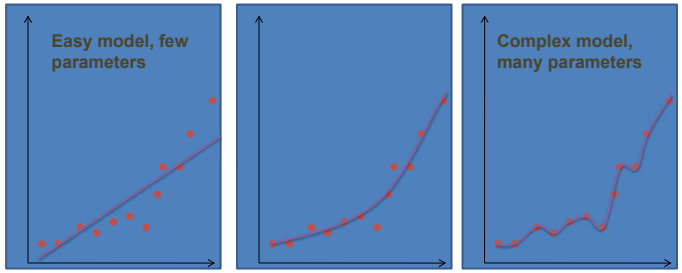
- Parametric models
  - Have certain number of parameters independently of the size of training data
  - Assumption about of the data distribution
  - Ex: logistic regression
- Nonparametric models
  - Number of parameters (complexity) grows with training data
    - Example: K-NN classifier





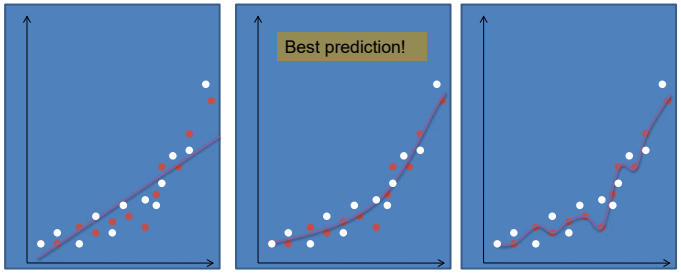
Overfitting

- Which model feels appropriate?



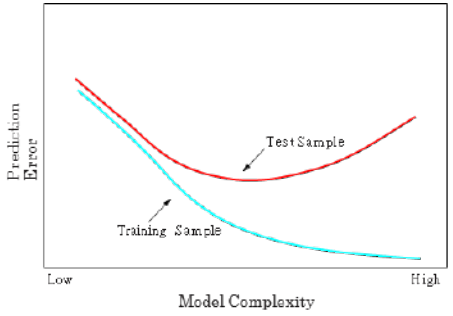
Overfitting

Now new data from the same process



Overfitting

- Observed:



Model selection

- Given several models $M_1, \dots M_m$
- Divide data set into **training** and **test** data

Training	Test

- Fit models M_i to training data→get parameter values
- Use fitted models to predict test data and compare **test errors** $R(M_1), \dots R(M_m)$
- Model with lowest prediction error is best

Comment:

- Approach works well for moderate/large data

Typical error functions

- Regression, **MSE** :

$$R(Y, \hat{Y}) = \frac{1}{N}\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$

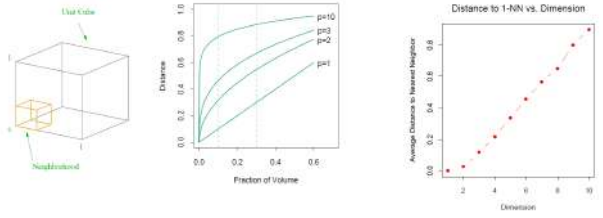
- Classification, **misclassification rate**

$$R(Y, \hat{Y}) = \frac{1}{N}\sum_{i=1}^{N} I(Y_i \neq \hat{Y}_i)$$

Curse of dimensionality

- Given data D:
  - Features $X_1, \dots X_p$
  - Targets $Y_1, \dots, Y_r$
- When p increases models using ”proximity” measures work badly
- Curse of dimensionality: A point has no ”near neighbors” in high dimensions → using class labels of a neighbor can be misleadning
  - Distance-based methods affected

Curse of dimensionality



Curse of dimensionality

- Hopeless? No!
- Real data normally has much lower effective dimension
  - Dimensionality reduction techniques
- Smoothness assumption
  - small change in one of Xs should lead to small change in Y→interpolation

Probability

How likely it is that some event will happen?

Idea:

- Experiment
- Outcomes (sample points) O_1, O_2,… O_n
- Sample space Ω
- Event A
- Probability function P: Events →[0,1]

Probability

Example: Tossing a coin two times

Example:

- $p(A)$ frequency of observing A
- $p(A,B)$ frequency of observing A and B
- $p(B|A)$ frequency of observing B given A

Properties and definitions

- One can think of events as sets
  - Set operations are defined: $A \cup B, A \cap B, \bar{A} \backslash B$
- $P(A \cup B) = P(A) + P(B)$ if $A \cap B = \emptyset$
- Independence $P(A,B) \equiv P(A \cap B) = P(A)P(B)$
- Conditional probability $P(A|B) = \frac{P(A,B)}{P(B)}$

Bayes theorem

Example:

- We have constructed spam filter that
  - identifies spam mail as spam with probability 0.95
  - Identifies usual mail as spam with probability 0.005
- This kind of spam occurs once in 100,000 mails
- If we found that a letter is a spam, what is the probability that it is actually a spam?

Bayes theorem

- We have some knowledge about event B
  - Prior probability P(B) of B
- We get new information A
  - P(A)
  - P(A|B) probability of A can occur given B has occured
- New (updated) knowledge about B
  - Posterior probability P(B|A)

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

Random variables

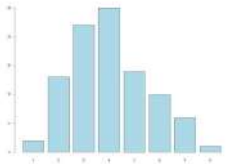
- Instead of having events, we can have a variable X:
  - Events→$\mathbb{R}$ Continuous random variables
  - Events→$\mathbb{N}$ Discrete random variables

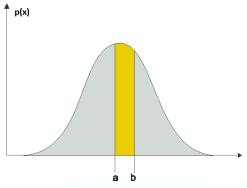
Examples:

- X={amount of times the word "crisis" can be found in financial documents}
  - P(X=3)
- X={Time to download a specific file to a specific computer}
  - P(X=0.36 min)

Distributions

- Discrete
  - Probability mass function P(x) for all feasible x
- Coninuous
  - Probability density function p(x)
    - $p(x \in [a,b]) = \int_a^b p(x)dx$
    - $p(x) \geq 0, \int_{-\infty}^{+\infty} p(x)dx = 1$
  - Cumulative distribution function $F(x) = \int_0^x p(t)dt$





Expected value and variance

- Expected value = mean value
  - $E(X) = \sum_{i=1}^{n} X_i P(X_i)$
  - $E(X) = \int Xp(X)dX$
- Variance how much values of random variable can deviate from mean value
  - $Var(X) = E\left(X - E(X)\right)^2 = E(X^2) - E(X)^2$

Probabilities

- **Laws of probabilities**
  - Sum rule (compute **marginal** probability)

$$p(X) = \sum_Y p(X,Y)$$

$$p(X) = \int p(X,Y)dY$$

  - Product rule

$$p(X,Y) = p(X|Y)p(Y)$$

Combination 1:

$$p(X) = \sum_Y p(X|Y)p(Y)$$

$$p(X) = \int p(X|Y)p(Y)dY$$

Bayes theorem

For random variables:

Bayes Theorem

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

$$p(Y|X) \propto p(X|Y)p(Y)$$

$$p(Y|X) = \frac{p(X|Y)p(Y)}{\int p(X|Y)p(Y)dY}$$

Some conventional distributions

Bernoulli distribution

- Events: Success (X=1) and Failure (X=0)
- P(X=1)=p, P(X=0)=1-p

- $E(X) = p$
- $Var(X) = 1 - p$

Examples: Tossing coin, vinning a lottery,..

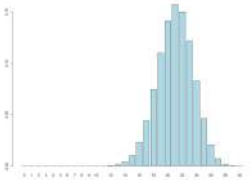
Some conventional distributions

Binomial distribution

- Sequence of *n* Bernoulli events
- X={Amount of successes among these events}, X=0,…,n

$$P(X = r) = \frac{n!}{(n-r)!\,r!} p^r (1-p)^{n-r}$$

- $EX = np$
- $Var(X) = np(1-p)$



Poisson distribution

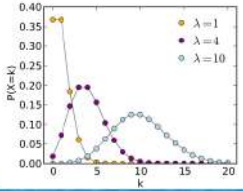
- Customers of a bank **n** (in theory, endless population)
- Probability that a specific person will make a call to the bank between 13.00 and 14.00 a certain day is ***p***
  - ***p*** can be very small if population is large (rare event)
  - Still, some people will make calls between 13.00 and 14.00 that day, and their amount may be quite big
  - A known quantity **λ=*np*** is mean amount of persons that call between 13.00 and 14.00
  - **X**={amount of persons that have called between 13.00 and 14.00}

Poisson distribution

- $P(X = r) = \lim_{n\to\infty} \frac{n!}{(n-r)!r!} p^r (1-p)^{n-r}$
- It can be shown that

$$P(X = r) = \frac{\lambda^r e^{-\lambda}}{r!}$$

- $E(X) = \lambda$
- $Var(X) = \lambda$



Poisson distribution

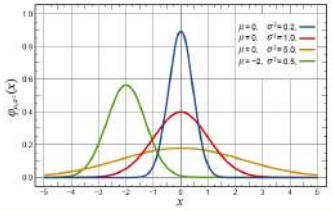
- Further properties:
  - Poisson distribution is a good approximation of the binomial distribution if n >20 and $p < 0.05$
  - Excellent approximation if $n \geq 100$ and $np \leq 10$

Normal distribution

- Appears in almost all applications
  - Difference between the times required to download two specific documents to a specific computer

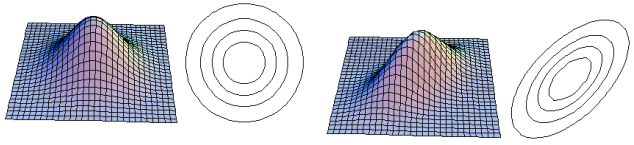
$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \sigma > 0$$

- $E(X) = \mu$
- $Var(X) = \sigma^2$



Multivariate distributions

- Probability of two variables having certain values at the same time
  - P.D.F. p(x,y)
  - Correlation



Basic ML ingridients

- Data D: observations
  - Features $X_1, \ldots X_p$
  - Targets $Y_1, \ldots, Y_r$

Case	X_1	X_2	Y
1			
2			
…			

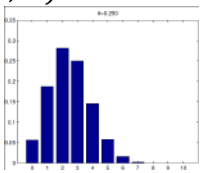
- Model $P(x|\, w_1, \ldots w_k)$ or $P(y|x, w_1, \ldots w_k)$
  - Example: Linear regression $p(y|x,w) = N(w_0 + w_1 x, \sigma^2)$
- Learning procedure (data→get parameters $\hat{w}$ or $p(w|D)$)
  - Maximum likelihood, Bayesian estimation
- Predict new data X^{new} by using the fitted model

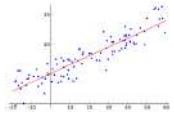
Probabilistic models

- A distribution $p(x|w)$ or $p(y|x,w)$
- Example:
  - $x \sim Bin(n,\theta)$

    $p(x=k|n,\theta) = \binom{n}{k}\theta^k(1-\theta)^{n-k}$

  - $y \sim N(\alpha_0 + \alpha_1 x, \sigma^2)$





Learn basic distributions and their properties→PRML, chapter 2!

Fitting a model

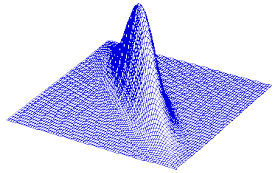
- Given dataset D and model $p(x|w)$ or $p(y|x,w)$
  - Frequentist approach: which combination of parameter values fits my data best?
  - Bayesian approach: parameters are random variables, all feasible values are acceptable
    - Different parameter values have different probabilities

Fitting a model

- Frequenist principle: **Maximum likelihood** principle
  - Compute likelihood $p(\boldsymbol{D}|\, w)$

$$p(\boldsymbol{D}|\, w) = \prod_{i=1}^{n} p(X_i|w)$$

$$p(\boldsymbol{D}|\, w) = \prod_{i=1}^{n} p(Y_i|X_i, w)$$



  - Maximize the likelihood and find the optimal w^*

Fitting a model

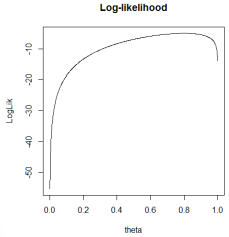
Remarks:

- Likelihood shows how much the chosen parameter value is proper for a specific model and the given data
- Normally **log-likelihood** is used in computations instead
- Other alternatives to ML exist…

Fitting a model

Example: tossing a coin.

$D = \{0,1,1,0,1,1,1,1,1,1,1,1\}$,
$p(x=1|\theta) = \theta, p(x=0|\theta) = 1-\theta$



Bayesian probabilities

- Probability reflects your knowledge (uncertainty) about a phenomenon → **subjective probabilities**
  - **Prior probability** $p(w)$, can be uninformative $p(w) \propto 1$
  - Formulate a model, compute **likelihood** $p(D|w)$
  - **Posterior probability** $p(w|D)$, after observing data
    - $p(w|D) \propto p(D|w)p(w)$
- Model parameters are considered as random variables
  - In real life, do not need to be random, but we model as random

Fitting a model

- Bayesian principle
  - Compute $p(w|D)$and then decide yourself what to do with this (for ex. MAP, mean, median)
- Use bayes theorem

$$p(w|D) = \frac{p(D|w)p(w)}{p(D)} \propto p(D|w)p(w)$$

- $p(D)$ is **marginal likelihood**
  - $p(D) = \int p(D|w)p(w)dw$ or
  - $p(D) = \sum_i p(D|w_i)p(w_i)$

Example: tossing a coin. Find $p(\theta|D)$, estimate posterior mean θ^*

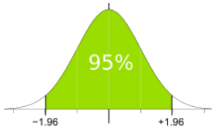
Fitting a model

- How to chose the prior?
  - Expert knowledge about the phenomenon
  - Forcing a model to have a certain structure
    - Example: decision trees: prior prefers smaller trees

      http://en.wikipedia.org/wiki/Conjugate_prior
  - Conjugacy
    - Distribution of the posterior is the same type as the distribution of the likelihood or prior
- Prior is the most controversial about Bayesian methods, but
  - When $N \to \infty$, data overwhelms the prior

Measuring uncertainty

- **Confidence interval** (frequentist)
  1. Model $p(x|w)$ is known
  2. $\hat{w}$ is a function of x by ML
  3. Derive distribution of $\hat{w}$
  4. Compute quantiles



- **Credible interval** (Bayes)
- **Prediction interval** (models)

- Example: Prediction interval for $Y \sim N(2x+4, 1)$ at $x = 5$

Regression and regularization

Lecture 1d

Overview

- Linear regression
- Ridge Regression
- Lasso
- Variable selection

Simple linear regression

Model:

$$y \sim N(w_0 + w_1 x, \sigma^2)$$

or

$$y = w_0 + w_1 x + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

or

$$p(y|x, w) = N(w_0 + w_1 x, \sigma^2)$$

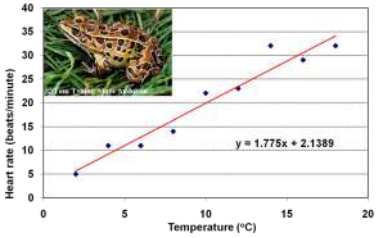
Terminology:

w_0: **intercept (or bias)**

w_1: **regression coefficient**

Response

The target responds directly and linearly to changes in the feature



Ordinary least squares regression (OLS)

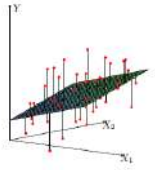
Model:

$$y \sim N(\boldsymbol{w}^T \boldsymbol{x}, \sigma^2)$$

where

$$\boldsymbol{w} = \{w_0, \ldots w_d\}$$
$$\boldsymbol{x} = \{1, x_1, \ldots x_d\}$$

Why is "1" here?



The response variable responds directly and linearly to changes in each of the inputs

Ordinary least squares regression

Given data set D

Case	X_1	X_2			X_p	Y
1	x_{11}	x_{21}			x_{p1}	y_1
2	x_{12}	x_{22}			x_{p2}	y_2
3	x_{13}	x_{23}			x_{p3}	y_3
N	x_{1N}	x_{2N}			x_{pN}	y_N

Estimation: maximizing the likelihood

$$\hat{w} = \max_w p(D|w)$$

Is equivalent to minimizing

$$RSS(w) = \sum_{i=1}^{n} (Y_i - \boldsymbol{w}^T \boldsymbol{X_i})^2$$

Matrix formulation of OLS regression

Optimality condition:

where $\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}) = 0$

$$\boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & x_{21} & & x_{p1} \\ 1 & x_{12} & x_{22} & & x_{p2} \\ & & & & \\ & & & & \\ 1 & x_{1N} & x_{2N} & & x_{pN} \end{pmatrix} \quad \textbf{and} \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \\ \\ y_N \end{pmatrix}$$

Parameter estimates and predictions

- Least squares estimates of the parameters

$$\hat{w} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

- Predicted values

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{w} = \boldsymbol{X}(\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y} = \boldsymbol{P}\boldsymbol{y}$$

- Linear regression belongs to the class of **linear smoothers**

Hat matrix

Why is it called so?

Degrees of freedom

Definition:

$$df(\hat{y}) = \frac{1}{\sigma^2} \sum_{i=1}^{N} Cov(\hat{y}_i, y_i)$$

- Larger covariance → stronger connection → model can approximate data better→ model more flexible (complex)
- For linear smoothers $\hat{Y} = S(X)Y$

$$df = trace(S)$$

- For linear regression, degrees of freedom is

$$df = trace(P) = p$$

Different types of features

- Interval variables
- Numerically coded ordinal variables
  - (small=1, medium=2, large=3)
- Dummy coded qualitative variables

Basis function expansion:
If $y = w_0 + w_1 x_1 + w_2 x_1^2 + w_3 e^{-x_2} + \epsilon$,

Model becomes linear if to recompute:

$$\phi_1(x_1) = x_1$$
$$\phi_2(x_1) = x_1^2$$
$$\phi_3(x_1) = e^{-x_2}$$

Example of dummy coding:

$$x_1 = \begin{cases} 1, \text{if Jan} \\ 0, \text{otherwise} \end{cases}$$

$$x_2 = \begin{cases} 1, \text{if Feb} \\ 0, \text{otherwise} \end{cases}$$

.
.
.

$$x_{11} = \begin{cases} 1, \text{if Nov} \\ 0, \text{otherwise} \end{cases}$$

Basis function expansion

- In general $\phi_1(\dots)$ may be a function of several x components
- Having data given by **X,** compute new data
- $\Phi = \begin{pmatrix} 1 & \phi_1(x_{11,}\dots,x_{1p}) & .. & \phi_p(x_{11,}\dots,x_{1p}) \\ & \dots & \dots & \dots \\ 1 & \phi_1(x_{n1,}\dots,x_{np}) & \dots & \phi_p(x_{n1,}\dots,x_{np}) \end{pmatrix}$
- If doing a basis function in a model, replace **X** by Φ everywhere where **X** is used:

$$\hat{y} = \Phi(\Phi^T\Phi)^{-1}\Phi^T y$$

Linear regression in R

- 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
```


An 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)
```

Response variable:
Requested price of used Porsche cars (1000 SEK)

```
> summary(fit1)

Call:
lm(formula = Price ~ Year, data = mydata)

Residuals:
    Min      1Q  Median      3Q     Max
-167683 -14683   20056   35933   72317

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -78161027    8448038  -9.252 6.00e-13 ***
Year            39246       4226   9.288 5.25e-13 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 57270 on 57 degrees of freedom
Multiple R-squared:  0.6021,    Adjusted R-squared:  0.5952
F-statistic: 86.26 on 1 and 57 DF,  p-value: 5.248e-13
```

Inputs:
X_1 = Manufacturing year
X_2 = Milage (km)
X_4 = Equipment (0 or 1)

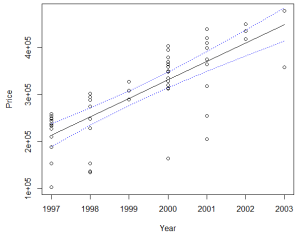
An example of ordinary least squares regression

```
> summary(fit2)

Call:
lm(formula = Price ~ Year + Mileage + Equipment, data = mydata)

Residuals:
   Min     1Q Median     3Q    Max
-66223 -10525   -739  14128  65332

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -2.083e+07  6.309e+06  -3.302  0.00169 **
Year         1.062e+04  3.154e+03   3.366  0.00139 **
Mileage     -2.077e+00  2.022e-01 -10.269 2.14e-14 ***
Equipment    5.790e+04  1.041e+04   5.563 8.08e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 29270 on 55 degrees of freedom
Multiple R-squared:  0.8997, Adjusted R-squared:  0.8942
F-statistic: 164.5 on 3 and 55 DF,  p-value: < 2.2e-16
```


An example of ordinary least squares regression

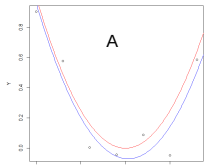
- Prediction

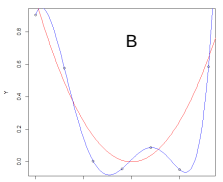
```
fitted <- predict(fit1, interval =
"confidence")

# 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

- Problem: linear regression can overfit:
  - Take $Y := Y, X_1 = X, X_2 = X^2, \dots, X_p = X^p$ → polinomial model, fit by linear regression
  - High degree of polynomial leads to overfitting.





Ridge regression

- **Idea**: Keep all predictors but shrink coefficients to make model less complex

minimize $-loglikelihood + \lambda_0\|w\|_2^2$

→ **l_2 regularization**

  - Given that model is Gaussian, we get **Ridge regression:**

$$\hat{w}^{ridge} = \text{argmin}\left\{\sum_{i=1}^{N}(y_i - w_0 - w_1x_{1j} - \dots - w_px_{pj})^2 + \lambda\sum_{j=1}^{p}w_j^2\right\}$$

- $\lambda > 0$ is **penalty factor**

Ridge regression

Equivalent form

$$\hat{w}^{ridge} = \text{argmin}\sum_{i=1}^{N}(y_i - w_0 - w_1x_{1j} - \dots - w_px_{pj})^2$$

subject to $\sum_{j=1}^{p}w_j^2 \le s$

Solution

$$\hat{\boldsymbol{w}}^{\boldsymbol{ridge}} = \left(\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{X} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{X}^{\boldsymbol{T}}\boldsymbol{y}$$

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{w}} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{P}\boldsymbol{y}$$

Hat matrix

How do we compute degrees of freedom here?

Ridge regression

Properties

- Extreme cases:
  - $\lambda = 0$ usual linear regression (no shrinkage)
  - $\lambda = +\infty$ fitting a constant ($w = 0$ except of w_0)
- When input variables are ortogonal (not realistic), $X^TX = I \rightarrow$

$$\hat{\boldsymbol{w}}^{\text{ridge}} = \frac{1}{1+\lambda}\mathbf{w}^{\mathbf{linreg}}$$ → coefficients are equally shrunk

- **Ridge regression is particularly useful if the explanatory variables are strongly correlated to each other.**
  - Correlated variables often correspond large w→shrunk
- Degrees of freedom decrease when λ increases
  - $\lambda = 0 \rightarrow d.f. = p$

Ridge regression

Properties

- Shrinking enables estimation of regression coefficients even if the number of parameters exceeds the number of cases! ($X^TX + \lambda I$ is always nonsingular)
  - Compare with linear regression
- How to estimate λ?
  - cross-validation

Ridge regression

- Bayesian view
  - Ridge regression is just a special form of Bayesian Linear Regression with constant σ^2:

$$y \sim N(y|w_o + Xw, \sigma^2 I)$$
$$w \sim N\left(0, \frac{\sigma^2}{\lambda} I\right)$$

Theorem MAP estimate to the Bayesian Ridge is equal to solution in frequenist Ridge

$$\hat{w}^{ridge} = \left(X^T X + \lambda I\right)^{-1} X^T y$$

- In Bayesian version, we can also make inference about λ

Ridge regression

Example Computer Hardware Data Set : performance measured for various processors and also

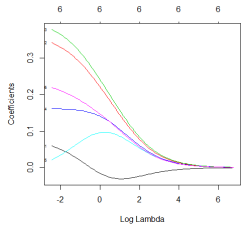
- Cycle time
- Memory
- Channels
- …

Build model predicting performance

Ridge regression

- R code: use package **glmnet** with alpha=0 (Ridge regression)
- Seeing how Ridge converges

```
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)
```

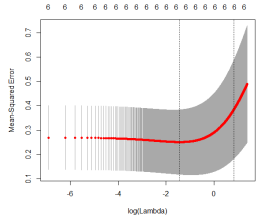


Ridge regression

- Choosing the best model by cross-validation:

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

```
> coef(model, s="lambda.min")
7 x 1 sparse Matrix of class "dgC
                      1
(Intercept) -4.530442e-17
V3           3.420739e-02
V4           3.085696e-01
V5           3.403839e-01
V6           1.593470e-01
V7           5.489116e-02
V8           1.970982e-01
```



> model$lambda.min
[1] 0.046

Ridge regression

- 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)
```

Note that data are so small so numbers change much for other train/test

```
> sum((ynew-mean(y))^2)/sum((y-mean(y))^2)
[1] 0.5438148
> sum((ynew-y)^2)
[1] 18.04988
>
```


LASSO

- **Idea**: Similar idea to Ridge
- Minimize minus loglikelihood plus **linear** penalty factor→ $\mathbf{l_1}$ **regularization**
  - Given that model is Gaussian, we get **LASSO** (least absolute shrinkage and selection operator):

$$\hat{w}^{lasso} = \operatorname{argmin}\left\{\sum_{i=1}^{N}(y_i - w_0 - w_1 x_{1j} - \ldots - w_p x_{pj})^2 + \lambda \sum_{j=1}^{p}|w_i|\right\}$$

- $\lambda > 0$ is **penalty factor**

LASSO

- Equivalently

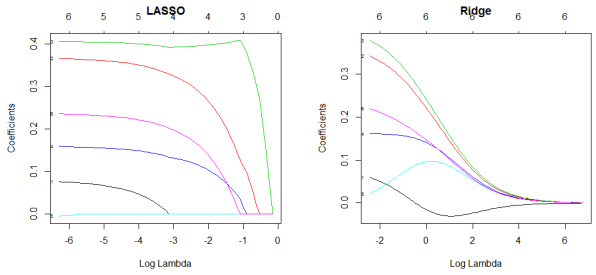
$$\hat{w}^{lasso} = \operatorname{argmin}\sum_{i=1}^{N}(y_i - w_0 - w_1 x_{1j} - \ldots - w_p x_{pj})^2$$

subject to $\sum_{j=1}^{p}|w_i| \le s$

LASSO vs Ridge

- **LASSO yields sparse solutions!**

Example Computer hardware data



LASSO vs Ridge

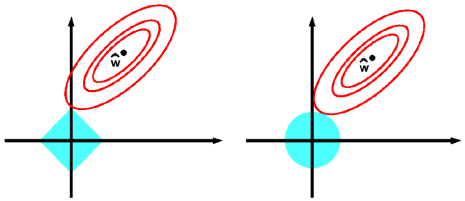
- Only 5 variables selected by LASSO

```
> coef(model, s="lambda.min")
7 x 1 sparse Matrix of class "dgCMatrix"
                      1
(Intercept) -5.091825e-17
V3           6.350488e-02
V4           3.578607e-01
V5           4.033670e-01
V6           1.541329e-01
V7           .
V8           2.287134e-01
> 
```

```
> sum((ynew-mean(y))^2)/sum((y-mean(y))^2)
[1] 0.5826904
> sum((ynew-y)^2)
[1] 16.63756
```


LASSO vs Ridge

- Why Lasso leads to sparse solutions?
  - Feasible area for Ridge is a circle (2D)
  - Feasible area for LASSO is a polygon (2D)



LASSO properies

- **Lasso is widely used when $p \gg n$**
  - Linear regression breaks down when $p > n$
  - Application: DNA sequence analysis, Text Prediction
- When inputs are orthonormal,

$$\hat{w}_i^{\text{lasso}} = sign(w_i^{linreg})\left(|w_i^{linreg}| - \frac{\lambda}{2}\right)_+$$

- No explicit formula for $\hat{w}^{lasso}$
  - Optimization algorithms used

Coding in R: use glmnet() with alpha=1

Variable selection

- .. Or “Feature selection”

Often, we do not need all features available in the data to be in the model

Reasons:

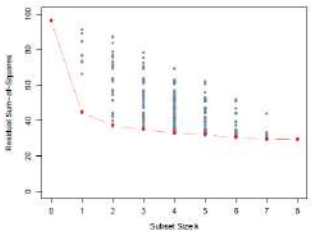
- Model can become overfitted (recall polynomial regression)
- Large number of predictors → model is difficult to use and interpret

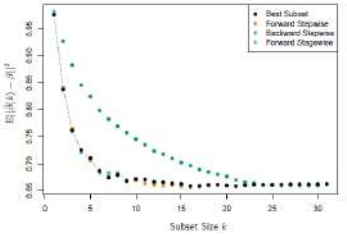
Variable selection

Alternative 1: Variable subset selection

- Best subset selection:
  - Consider different subsets of the full set of features, fit models and evaluate their quality
    - Problem: computationally difficult for p around 30 or more
    - How to choose the best model size? Some measure of predictive performance normally used (ex. AIC).
- Forward and Backward stepwise selection
  - Starts with 0 features (or full set) and then adds a feature (removes feature) that most improves the measure selected.
    - Can handle large *p* quickly
    - Does not examine all possible subsets (not the “best”)

RSS and MSE depend on k





Variable selection in R

- Use stepAIC() in MASS

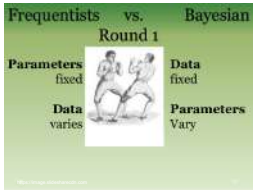
```
library(MASS)
fit <- lm(V9~.,data=data.frame(data1))
step <- stepAIC(fit, direction="both")
step$anova
summary(step)
```

```
Call:
lm(formula = V9 ~ V3 + V4 + V5 + V6 + V8, data = data.fra

Residuals:
     Min       1Q   Median       3Q      Max
-1.20232 -0.15512  0.03579  0.16567  2.42280

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -5.783e-17  2.574e-02   0.000   1.0000
V3           7.948e-02  2.826e-02   2.813   0.0054 **
V4           3.661e-01  4.312e-02   8.490 4.34e-15 ***
V5           4.055e-01  4.664e-02   8.695 1.18e-15 ***
V6           1.591e-01  3.394e-02   4.687 5.07e-06 ***
V8           2.360e-01  3.356e-02   7.031 3.06e-11 ***
```

```
> step <- stepAIC(fit, direction="both")
Start:  AIC=-405.35
V9 ~ V3 + V4 + V5 + V6 + V7 + V8

       Df Sum of Sq     RSS     AIC
- V7    1    0.0139 28.117 -407.25
<none>              28.103 -405.35
- V3    1    1.0819 29.185 -399.46
- V6    1    2.9385 31.041 -386.57
- V8    1    6.3150 34.418 -364.99
- V4    1    9.7492 37.852 -345.11
- V5    1   10.4837 38.586 -341.09

Step:  AIC=-407.25
V9 ~ V3 + V4 + V5 + V6 + V8

       Df Sum of Sq     RSS     AIC
<none>              28.117 -407.25
+ V7    1    0.0139 28.103 -405.35
- V3    1    1.0958 29.212 -401.26
- V6    1    3.0431 31.160 -387.77
- V8    1    6.8472 34.964 -363.70
- V4    1    9.9840 38.101 -345.74
- V5    1   10.4713 38.588 -343.08
```

Frequentist vs Bayesian

- Probabilistic Model $p(y, x, w)$
  - **Frequentists**: w is a parameter that should be estimated by model fitting
  - **Bayesians**: w is a random variable that has a prior distribution $p(w)$
    - How to set $p(w)$??



Example: Linear regression, what are parameters here?

$y \sim w_0 + \boldsymbol{wx} + e, e \sim N(0, \sigma^2)$

$y \sim N(w_0 + \boldsymbol{wx}, \sigma^2)$

An estimator

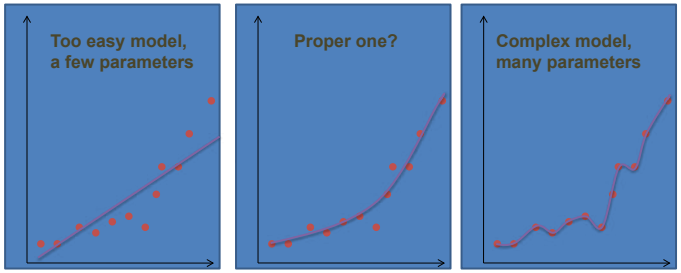
- $\widehat{\boldsymbol{w}} = \delta(D)$ (some function of your data) – an **estimator**
- Optimal parameter values?→there can be many ways to compute them (MLE, shrinkage…)
  - Compare Bayesian: given estimators $\boldsymbol{w^1}$ and $\boldsymbol{w^2}$, we **can** compare them! $p(\boldsymbol{w^1}|\boldsymbol{D}) > \boldsymbol{p}(\boldsymbol{w^2}|\boldsymbol{D})$
  - There is no easy way to compare estimators in frequentist tradition

Example: Linear regression

- Estimator 1: $\boldsymbol{w} = (X^T X)^{-1} X^T Y$ (maximum likelihood)
- Estimator 2: $\boldsymbol{w} = (0, \dots, 0, 1)$
- Which one is better?
  - A comparison strategy is needed!

Overfitting

- Complex model can overfit your data



Overfitting: solutions

- Observed: Maximum likelihood can lead to overfitting.
- Solutions
  - Selecting proper parameter values
    - Regularized risk minimization
  - Selecting proper model type, for ex. number of parameters
    - Houldout method
    - Cross-validation

Model selection

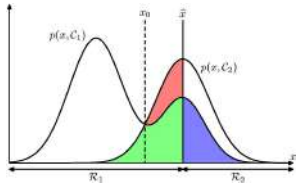
- Given a model, choose the optimal parameter values
  - Decision theory
- Define loss $L(Y, \hat{y})$
  - How much we loose in guessing true Y incorrectly
- If we know the true distribution $p(y, x|w)$ then we choose $\hat{y}$

$$\min_{\hat{y}} EL(y, \hat{y}) = \min_{\hat{y}} \int L(y, \hat{y}) p(y, x|w) dx dy$$

Model selection

Example: Spam classification

- Loss for incorrect classifying mails and spams
  - $L_{12} = 100, L_{21} = 1$



Loss functions

- How to define loss function?
  - No unique choice, often defined by application
  - **Normal practice: Choose the loss related to minus loglikelihood**

Example: Predicting the amount of the product at the storage:

$$L(Y, \hat{y}) = \begin{cases} 10 - \frac{\hat{y}}{Y}, \hat{y} \le Y \\ 1000, \hat{y} > Y \end{cases}$$

Example: Compute loss function related to

- Normal distribution

Guess why such loss function was chosen

Loss functions

- Classification problems
  - Common loss function $L(Y, \hat{y}) = \begin{cases} 0, Y = \hat{y} \\ 1, Y \neq \hat{y} \end{cases}$
  - When minimizing the loss, equivalent to misclassification rate

Model selection

- **Problem**: true model and true $\boldsymbol{w}$ are unknown→can not compute expected loss!
- How to find an optimal model?
  - Consider what expected loss (**risk**) depends on

$$R(Y, \hat{y}) = E[L(Y, \hat{y}(X, D))]$$

- Random factors:
  - D – **training set**
  - Y, X – data to be predicted **(validation set)**

Holdout method

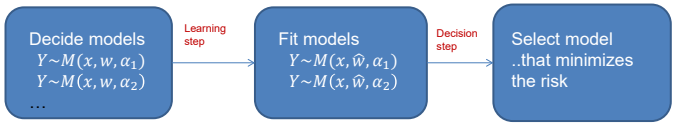
- Simplify the risk estimation:
  - Fix D as a particular training set T
  - Fix Y,X as a particular validation set V
- Risk becomes (**empirical risk**)

$$\hat{R}(y,\hat{y}) = \frac{1}{|V|}\sum_{(X,Y)\in V} L(Y,\hat{y}(X,T))$$

  - Estimator is fit by Maximum Likelihood using training set
  - Risk estimated by using validation set
  - Model with minimum empirical risk is selected

General model selection strategy

- Given data $D = \{\boldsymbol{X}_i, Y_i, i = 1 \dots n\}$



- When fitting data, Maximum Likelihood is usually used
- α_i can be different things:
  - Type of distribution
  - Number of variables in the model
  - Regulatization parameter value
  - …

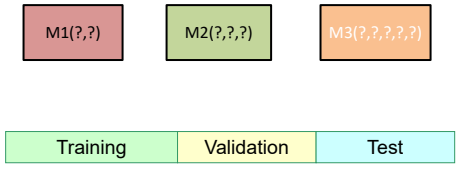
Holdout method

Divide into training, validation and test sets

- Choose proportions in some way

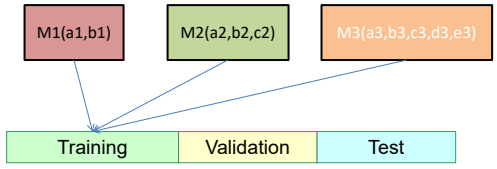
Holdout method

- Given: training, validation, test sets and models to select between



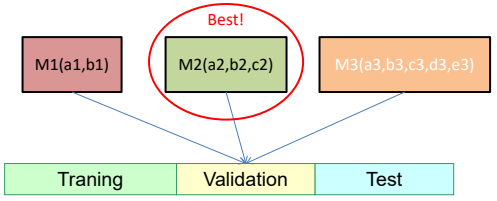
Holdout method

- Training set is to used for fitting models to the dataset by using maximum likelihood



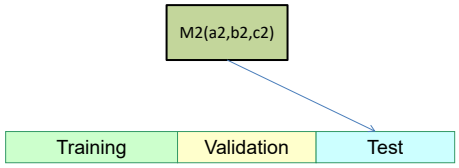
Holdout method

- Validation set is used to choose the best model (lowest risk)

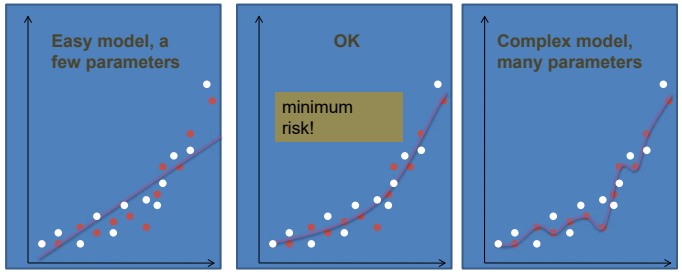


Holdout method

- Test set is used to test a performance on a new data



Holdout method



Holdout in R

- How to partition into train/test?
  - Use set.seed(12345) in the labs to get identical results

```
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,]
```

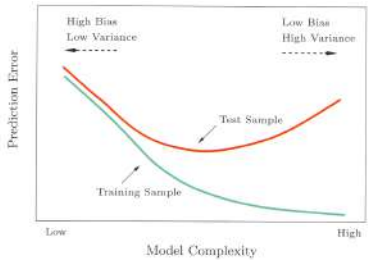
Bias-variance tradeoff

- Bias of an estimator $Bias(\hat{y}\ (x_0)) = E[\hat{y}(x_0) - f(x_0)]$, $f(x_0)$ is expected response
  - If $Bias(\hat{y}(x_0)) = 0$, the estimator is **unbiased**
  - ML estimators are asymptotically unbiased if the model is enough complex
  - However, unbiasedness does not mean a good choice!

Bias-variance tradeoff

- Assume loss is $L(Y, \hat{y}) = (Y - \hat{y})^2$

$$R(Y(x_0), \hat{y}(x_0)) = \sigma^2 + Bias^2(\hat{y}(x_0)) + Var(\hat{y}(x_0))$$



When loss is not quadratic, no such nice formula exist

Cross-validation

- Compared to holdout method:
  - Why do we use only some portion of data for training- can we use more (increase accuracy)?

Cross-validation (Estimates Err)

K-fold cross-validation (rough scheme, show picture):

1. Permute the observations randomly
2. Divide data-set in K roughly equally-sized subsets
3. Remove subset #i and fit the model using remaining data.
4. Predict the function values for subset #i using the fitted model.
5. Repeat steps 3-4 for different i
6. CV= squared difference between observed values and predicted values (another function is possible)

Cross-validation

Cross-validation

Note: if K=N then method is *leave-one-out* cross-validation.

$$\kappa : \{1, \ldots, N\} \mapsto \{1, \ldots, K\}$$

K-fold cross-validation: $CV = \frac{1}{N}\sum_{i=1}^{N} L(Y_i, \hat{y}^{-k(i)}(x_i))$

What to do if N is not a multiple of K?

Cross-validation vs Holdout

- Holdout is easy to do (a few model fits to each data)
- Cross validation is computationally demanding (many model fits)
- Holdout is applicable for large data
  - Otherwise, model selection performs poorly
- Cross validation is more suitable for smaller data

Analytical methods

- Analytical expressions to select models
  - AIC (Akaike's information criterion)

Idea: Instead of $R(Y, \hat{y}) = E[L(Y, \hat{y}(X, D))\ ]$ consider **in-sample** risk (only *Y* in *D* is random):

$$R_{in}(Y, \hat{y}) = \frac{1}{N}\sum_{i=1}^{N} E_{Y_i}\left[L\left(Y_i, \hat{y}(X, D)\right) | D, X \in D\right]$$

Analytical methods

- One can show that

$$R_{in}(Y, \hat{y}) \approx R_{train} + \frac{2}{N}\sum_{i} cov(\hat{y}_i, Y_i)$$

where $R_{train} = \frac{1}{N}\sum_{X_i Y_i \in T} L(Y_i, \hat{y}_i)$

- Recall, **degrees of freedom** $\mathrm{df(model)} = \frac{1}{\sigma^2}\sum_i cov(\hat{y}_i, Y_i)$
  - When model is linear, *df* is the number of parameters.
- If loss is defined by minus two loglikelihood,

$$AIC \equiv -2loglik(D) + 2df(model)$$

Model selection

Example Computer Hardware Data Set : performance measured for various processors and also

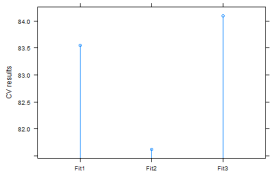
- Cycle time
- Memory
- Channels
- …

Build model predicting performance

Cross-validatation

- 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)
```



Linear classification methods

Lecture 2a

Overview

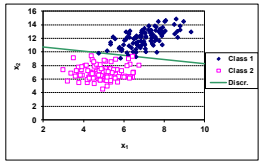
- Elements of decision theory
- Logistic regression
- Discriminant Analysis models

Classification

- Given data $D = \left((X_i, Y_i), i = 1 \dots N\right)$
  - $Y_i = Y(X_i) = C_j \in \boldsymbol{C}$
  - Class set $\boldsymbol{C} = (C_1, \dots, C_K)$

Classification problem:

- Decide $\hat{Y}(x)$ that maps **any** x into some class C_K
  - Decision boundary



Classifiers

- **Deterministic**: decide a rule that directly maps X into $\hat{Y}$
- **Probabilistic:** define a model for $P(Y = C_i|X), i = 1 \dots K$

Disanvantages of deterministic classifiers:

- Sometimes simple mapping is not enough (risk of cancer)
- Difficult to embed loss-> rerun of optimizer is often needed
- Combining several classifiers into one is more problematic
  - Algorithm A classifies as spam, Algorithm B classifies as not spam → ???
  - P(Spam|A)=0.99, P(Spam|B)=0.45 → better decision can be made

Bayesian decision theory

- Machine learning models estimate $p(y|x)$ or $p(y|x, \hat{w})$
- Transform probability into action→ which value to predict?→decision step
  - $p(Y = Spam|x) = 0.83$→do we move the mail to Junk?
  - What is more dangerous: deleting 1 non-spam mail or letting 1 spam mail enter Inbox?
- →**Loss function** or **Loss matrix**

Loss matrix

- Costs of classifying $Y = C_k$ to C_j:
  - Rows: true, columns: predicted

$$L = \|L_{ij}\|, i = 1, \dots, n, j = 1, \dots, n$$

- Example 1: 0/1-loss

$$L = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

- Example 2: Spam

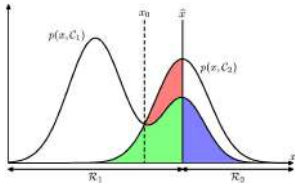
$$L = \begin{pmatrix} 0 & 100 \\ 1 & 0 \end{pmatrix}$$

Loss and decision

- Expected loss minimization
  - R_j : classify to C_j

$$EL = \sum_k \sum_j \int_{R_j} L_{kj} p(\boldsymbol{x}, C_k) d\boldsymbol{x}$$

- **Choose such R_j that EL is minimized**
- Two classes

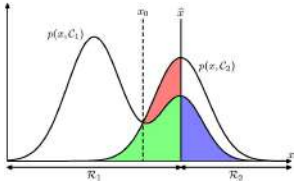


$$EL = \int_{R_1} L_{21} p(x, C_2) dx + \int_{R_2} L_{12} p(x, C_1)\, dx$$

Loss and decision

- Loss minimization

$$\min_{\hat{y}} EL(y, \hat{y}) = \min_{f} \int L(y, \hat{y}) p(y, x|w) dx dy$$



When loss is
$\begin{cases} 1, wrongly\ classified \\ 0, correctly\ classified \end{cases}$

Classify Y as
$\hat{Y} = \arg\max_c p(Y = c|X)$

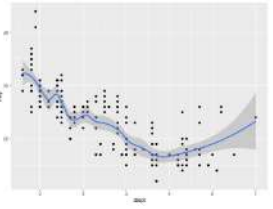
Loss and decision

- How to minimize *EL with two classes?*
- Rule:
  - $L_{12} p(x, C_1) > L_{21} p(x, C_2)$ →predict y as C_1
- 0/1 Loss: classify to the class which is more probable!

$$\frac{p(C_1|x)}{p(C_2|x)} > \frac{L_{21}}{L_{12}} \rightarrow predict\ y\ as\ C_1$$

Loss and decision

- Continuous targets: squared loss
  - Given a model $p(x,y)$, minimize
    $EL = \int L\left(y, \hat{Y}(x)\right) p(x,y)dxdy$
- Using **square loss**, the optimal is posterior mean
  $\hat{Y}(x) = \int yp(y|x)dy$



ROC curves

- Binary classification
- The choice of the thershold $\hat{x} = \frac{L_{21}}{L_{12}}$ affects prediction→ what if we don't know the loss? Which classifier is better?
- **Confusion matrix**

		PREDICTED		
		1	0	Total
TRUE	1	TP	FN	N_+
	0	FP	TN	N_-

ROC curves

- **True Positive Rates** (TPR) = **sensitivity** = **recall**
  - Probability of detection of positives: TPR=1 positives are correctly detected

$$TPR = TP/N_+$$

- **False Positive Rates** (FPR)
  - Probability of false alarm: system alarms (1) when nothing happens (true=0)

$$FPR = FP/N_-$$

- **Specificity**

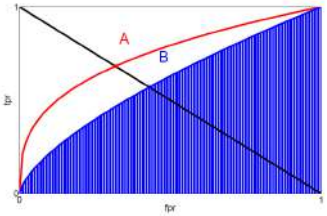
$$Specificity = 1 - FPR$$

- **Precision**

$$Precision = \frac{TP}{TP + FP}$$

ROC curves

- **ROC**=Receiver operating characteristics
- Use various thresholds, measure TPR and FPR
- Same FPR, higher TPR→ better classifier
- Best classifier = greatest Area Under Curve (**AUC**)



Types of supervised models

- **Generative models**: model $p(X|Y,w)$and $p(Y|w)$
  - Example: k-NN classification

$$p(X = x|Y = C_i, K) = \frac{K_i}{N_i V}, p(C_i|K) = \frac{N_i}{N}$$

From Bayes Theorem,

$$p(Y = C_i|x, K) = \frac{K_i}{K}$$

- **Discriminative models**: model $p(Y|X,w)$, X constant
  - Example: logistic regression
  - $p(Y = 1|\boldsymbol{w}, \boldsymbol{x}) = \frac{1}{1+e^{-\boldsymbol{w}^T\boldsymbol{x}}}$

Generative vs Discriminative

- Generative can be used to generate new data
- Generative normally easier to fit (check Logistic vs K-NN)
- Generative: each class estimated separately→ do not need to retrain when a new class added
- Discriminative models: can replace X with $\phi(X)$ (preprocessing), method will still work
  - Not generative, distribution will change
- Generative: often make too strong assumptions about $p(X|Y,w)$ → bad performance

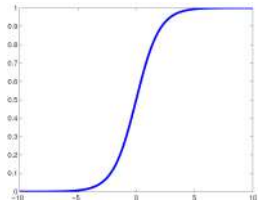
Logistic regression

- Discriminative model
- Model for binary output
  - $C = \{C_1 = 1, C_2 = 0\}$
    $p(Y = C_1|X) = sigm(\boldsymbol{w}^T\boldsymbol{x})$

$$sigm(a) = \frac{1}{1+e^{-a}}$$

- Alternatively
  $Y \sim Bernoulli(sigm(a)), a = \boldsymbol{w}^T\boldsymbol{x}$
  $sigm(a) = \frac{1}{1+e^{-a}}$

What is $P(Y = C_2|X)$?



Logistic regression

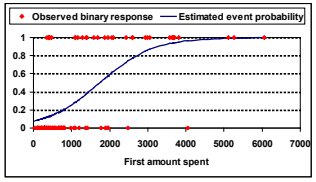
- Logistic model- yet another form

$$ln\frac{p(Y=1|X=x)}{P(Y=0|X=x)} = ln\frac{p(Y=1|X=x)}{1-P(Y=1|X=x)} = logit(p(Y=1|X=x)) = \boldsymbol{w}^T\boldsymbol{x}$$

The log of the odds is linear in *x*

- Here $logit(t) = \ln\left(\frac{t}{1-t}\right)$
- Note $p(Y|X)$ is connected to $\boldsymbol{w}^T\boldsymbol{x}$ via logit link

Example: Probability to buy more than once as function of First Amount Spend

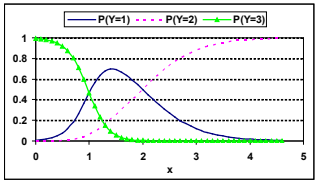


Logistic regression

- When Y is categorical,

$$p(Y = C_i|x) = \frac{e^{\boldsymbol{w}_i^T\boldsymbol{x}}}{\sum_{j=1}^{K} e^{\boldsymbol{w}_j^T\boldsymbol{x}}} = softmax(\boldsymbol{w}_i^T\boldsymbol{x})$$

- Alternatively
  $Y \sim Multinoulli\left(softmax(\boldsymbol{w}_1^T\boldsymbol{x}), \ldots softmax(\boldsymbol{w}_K^T\boldsymbol{x})\right)$



Logistic regression

Fitting logistic regression

- In binary case,

$$\log P(D|w) = \sum_{i=1}^{N} y_i \log(sigm(w^T x_i)) + (1 - y_i)\log(1 - sigm(w^T x_i))$$

  - Can not be maximized analytically, but unique maximizer exists
- To maximize loglikelihood, optimization used
  - Newton's method traditionally used (Iterative Reweighted Least Squares)
  - Steepest descent,Quasi-newton methods…

Estimation:

For new x, estimate $p(y) = [p_1, \dots p_C]$ and classify as $\arg \max_i p_i$

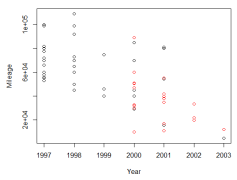
Decision boundaries of logistic regression are linear

Logistic regression

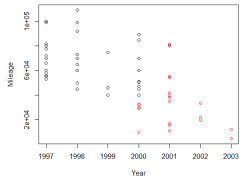
- In R, use glm() with family="binomial"
  - Predicted probabilities: predict(fit,newdata, type="response")

Example Equipment=f(Year, mileage)

Original data



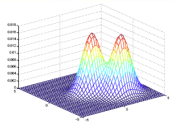
Classified data



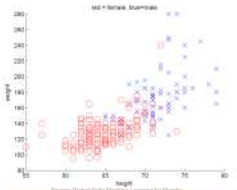
Quadratic discriminant analysis

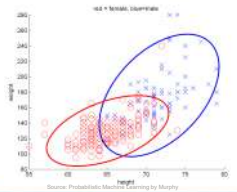
- Generative classifier
- Main assumptions:
  - $\boldsymbol{x}$ is now **random** as well as y

$$p(\boldsymbol{x}|y = C_i, \theta) = N(\boldsymbol{x}|\boldsymbol{\mu_i}, \boldsymbol{\Sigma_i})$$



Unknown parameters $\boldsymbol{\theta} = \{\boldsymbol{\mu_i}, \boldsymbol{\Sigma_i}\}$

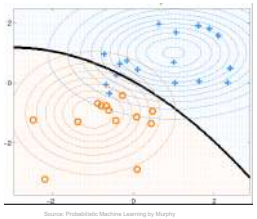




Quadratic discriminant analysis

- If parameters are estimated, classify:

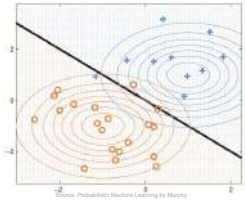
$$\hat{y}(\boldsymbol{x}) = \arg\max_c p(y = c|\boldsymbol{x}, \theta)$$



Linear discriminant analysis (LDA)

- Assumtion $\Sigma_i = \Sigma, i = 1, \dots K$
- Then $p(y = c_i|x) = softmax(w_i^T x + w_{0i})$ →exactly the same form as the logistic regression
  - $w_{0i} = -\frac{1}{2}\boldsymbol{\mu}_i^T \Sigma^{-1} \boldsymbol{\mu}_i + \log \pi_i$
  - $w_i = \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_i$
- Decision boundaries are linear
  - **Discriminant function**:

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



Linear discriminant analysis (LDA)

- Difference LDA vs logistic regression??
  - Coefficients will be estimated differently! (models are different)
- How to estimate coefficients
  - find MLE.

$$\hat{\mu}_c = \frac{1}{N_c} \sum_{i:y_i=c} \mathbf{x}_i, \quad \hat{\Sigma}_c = \frac{1}{N_c} \sum_{i:y_i=c} (\mathbf{x}_i - \hat{\mu}_c)(\mathbf{x}_i - \hat{\mu}_c)^T$$

$$\hat{\Sigma} = \frac{1}{N} \sum_{c=1}^{k} N_c \hat{\Sigma}_c$$

  - Sample mean and sample covariance are MLE!
  - If class priors are parameters (**proportional priors**),

$$\hat{\pi}_c = \frac{N_c}{N}$$

LDA and QDA: code

- Syntax in R, library **MASS**

lda(formula, data, ..., subset, na.action)
- Prior – class probabiliies
- Subset – indices, if training data should be used

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

predict(..)

LDA: output

```
resLDA=lda(Equipment~Mileage+Year, data=mydata)
 print(resLDA)
```

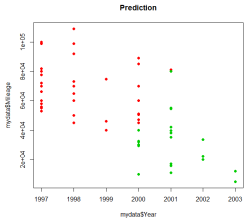
```
> print(resLDA)
Call:
lda(Equipment ~ Mileage + Year, data = mydata)

Prior probabilities of groups:
        0         1
0.6440678 0.3559322

Group means:
   Mileage     Year
0 63539.21 1998.447
1 36857.62 2000.762

Coefficients of linear discriminants:
                LD1
Mileage -1.500069e-05
Year     5.745893e-01
```


LDA: output

- Misclassified items

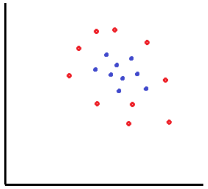
```
plot(mydata$Year, mydata$Mileage,
col=as.numeric(Pred$class)+1, pch=21,
bg=as.numeric(Pred$class)+1,
main="Prediction")
```

```
> table(Pred$class, mydata$Equipment)

    0  1
 0 31  6
 1  7 15
```



LDA versus Logistic regression

- Generative classifiers are easier to fit, discriminative involve numeric optimization
- LDA and Logistic have same model form but are fit differently
- LDA has stronger assumptions than Logistic, some other generative classifiers lead also to logistic expression
- New class in the data?
  - Logistic: fit model again
  - LDA: estimate new parameters from the new data
- Logistic and LDA: complex data fits badly unless interactions are included



LDA versus Logistic regression

- LDA (and other generative classifiers) handle missing data easier
- Standardization and generated inputs:
  - Not a problem for Logistic
  - May affect the performance of the LDA in a complex way
- Outliers affect Σ → LDA is not robust to gross outliers
- LDA is often a good classification method even if the assumption of normality and common covariance matrix are not satisfied.

Naïve Bayes classifiers
Decision trees

Lecture 2b

Naive Bayes classifiers: motivation

- Consider n labeled text documents
  - $Y = \{0,1\},\ 0 =$ "$Science\ fiction$", $1 =$ "$Comedy$"
  - $X = \{X_1, \dots X_{100}\}$ does the document contain the keyword (0=No,1=Yes)
    - X_1 corr. "space", X_2 corr. "fun",...

- Want to classify a new document

Naive Bayes classifiers: motivation

Idea: use Bayes classifier

$$p(Y = y|X) = \frac{P(X|Y = y)P(Y = y)}{\sum_j P(X|Y = y_j)P(Y = y_j)}$$

Chance of observing a given combination of words in science fiction

Proportion of science fiction documents

Naive Bayes classifiers: motivation

- Attempt 1:
  - Model $P(X = (x_1, \dots x_p)|Y = y_i)$ and $P(Y = y_i)$ as unknown parameters
  - Use data to derive those with Maximum Likelihood
  - Classify by use of the posterior distribution
- How many parameters?
  - How many different combinations of X? 2^p
  - Amount of $P(X = (x_1, \dots x_p)|Y = y_i)$ is $2 * 2^p - 2$
    - Probabilities for each Y sum up to one
- If $p = 100$, 10^{30} parameters need to be estimated→ ouch!

Naive Bayes classifiers

- Naive Bayes assumption: conditional independence

$$P(X = (x_1, \dots x_p)|Y = y) = \prod_{i=1}^{p} P(X_i = x_i|Y = y)$$

- How many parameters now?
  - $P(X_i = x_i|Y = y), i = 1, \dots p, x_i = \{0,1\}, y = \{0,1\}$ $2 * p$
- Is Naive Bayes assumption always valid?
  - P(Space,ship|SciFi)= P(Space|SciFi)*P(Ship|SciFi) ?

Naive Bayes classifiers - discrete inputs

- Given $D = \{(X_{m1}, \dots X_{mp}, Y_m),\ m = 1, \dots n\}$
- Assume $X_i \in \{x_1, \dots x_j\}, i = 1, \dots p, Y \in \{y_1 \dots y_K\}$
- Denote $\theta_{ijk} = p(X_i = x_j|Y = y_k)$
  - How many parameters? $(J-1)Kp$
- Denote $\pi_k = p(Y = y_k)$
- Maximum likelihood: assume θ_{ijk} and π_k are constants
  - $\hat{\theta}_{ijk} = \frac{\#\{X_i = x_j \,\&\, Y = y_k\}}{\#\{Y = y_k\}}$
  - $\hat{\pi}_k = \frac{\#\{Y = y_k\}}{n}$
  - Classification using 0-1 loss: $\hat{Y} = \arg\max_y p(Y = y|X)$

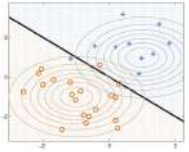
Naive Bayes classifiers - discrete inputs

- **Example** Loan decision
  - Classify a person: Home Owner=No, Single=Yes

Tid	Home Owner	Marital Status	Annual Income	Defaulted Borrower
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Naive Bayes – continuous inputs

- X_i are continuous
- Assumption A: $x_j|y = C$ are univariate Gaussian
  - $p(x_j|y = C_i, \theta) = N(x_j|\mu_{ij}, \sigma_{ij}^2)$
- Therefore $p(\boldsymbol{x}|y = C_i, \theta) = N(\boldsymbol{x}|\boldsymbol{\mu_i}, \boldsymbol{\Sigma_i})$
  - $\boldsymbol{\Sigma_i}$=diag$(\sigma_{i1}^2, \dots, \sigma_{ip}^2)$

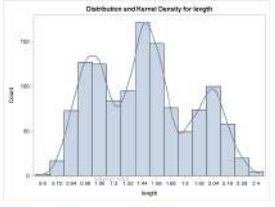


- Naive bayes is a special case of LDA (given A)
  - →MLE are means and variances (per class)

Naive Bayes – continuous inputs

- Assumption B: $p(x_j|y = C)$ are unknown functions of x_j that can be estimated from data
  - Nonparametric density estimation (kernel for ex.)

1. Estimate $p(X_i = x_j|Y = y_k)$ using nonparametric methods
2. Estimate $p(Y = y_k)$ as class proportions
3. Use Bayes rule and 0-1 loss to classify



Naive Bayes in R

- naiveBayes in package **e1071**

Example: Satisfaction of householders with their present housing circumstances

```
library(MASS)
library(e1071)
n=dim(housing)[1]
ind=rep(1:n, housing[,5])
housing1=housing[ind,-5]

fit=naiveBayes(Sat~., data=housing1)
fit

Yfit=predict(fit, newdata=housing1)
table(Yfit,housing1$Sat)
```

```
> table(Yfit,housing1$Sat)

Yfit      Low Medium High
  Low     294    162  144
  Medium  20     23   20
  High    253    261  504
```

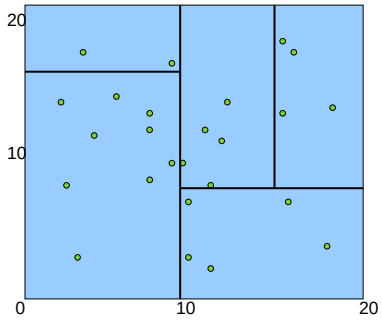

Decision trees

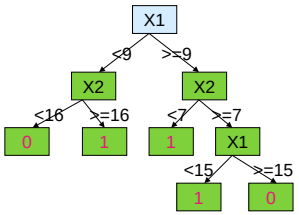
Idea

Split the domain of feature set into the set of hypercubes (rectangles, cubes) and define the target value to be constant within each hypercube

- Regression trees:
  - Target is a continuous variable
- Classification trees
  - Target is a class (qualitative) variable

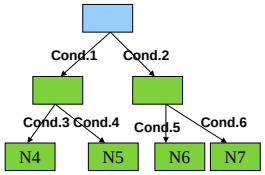
Classification tree toy example



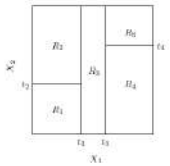


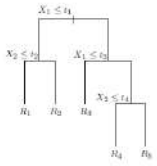
Definitions

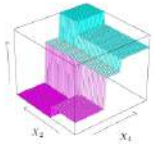
- Root node
- Nodes
- Leaves (terminal nodes)
- Parent node, child node
- Decision rules
- A value is assigned to the leaves



Regression tree toy example







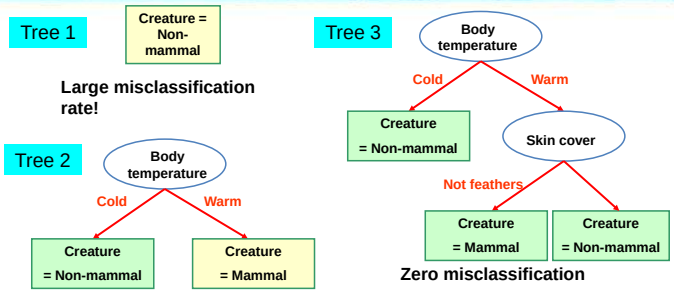
A classification problem

Create a classification tree that would describe the following patterns

ID	x1	x2	x3	x4	x5	x6	x7	y

Name	Body temperature	Skin cover	Gives birth	Aquatic creature	Aerial creature	Has legs	Hibernates	Class label
human	warm-blooded	hair	yes	no	no	yes	no	mammal
python	cold-blooded	scales	no	no	no	no	yes	non-mammal
salmon	cold-blooded	scales	no	yes	no	no	no	non-mammal
whale	warm-blooded	hair	yes	yes	no	no	no	mammal
frog	cold-blooded	none	no	semi	no	yes	yes	non-mammal
komodo	cold-blooded	scales	no	no	no	yes	no	non-mammal
bat	warm-blooded	hair	yes	no	yes	yes	yes	mammal
pigeon	warm-blooded	feathers	no	no	yes	yes	no	non-mammal
cat	warm-blooded	fur	yes	no	no	yes	no	mammal
shark	cold-blooded	scales	yes	yes	no	no	no	non-mammal
turtle	cold-blooded	scales	no	semi	no	yes	no	non-mammal
penguin	warm-blooded	feathers	no	semi	no	yes	no	non-mammal
porcupine	warm-blooded	quills	yes	no	no	yes	yes	mammal
eel	cold-blooded	scales	no	yes	no	no	no	non-mammal
salamander	cold-blooded	none	no	semi	no	yes	yes	non-mammal

Several solutions



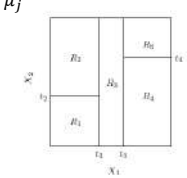
Green boxes represent pure nodes =nodes where observed values are the same

Decision trees

- A tree $T =< r_i, s_{r_i}, R_j, i = 1 \dots S, j = 1 \dots L >$
  - $x_{r_i} \leq s_{r_i}$ splitting rules (conditions), S- their amount
  - R_j-terminal nodes, L- their amount
  - labels μ_j in each terminal node

Model:

- $Y|T$ for R_j comes from exponential family with mean μ_j
- Fitting by MLE:
  - Step 1: Finding optimal tree
  - Step 2: Finding optimal labels in terminal nodes



Decision trees

Example:

- **Normal model** leads to regression trees
  - Objective: MSE
- **Multinoulli model** leads to classification trees
  - Objective: cross-entropy (deviance)

Classification trees

- Target is categorical
- Classification probability $p_{mk} = p(Y = k|X \in R_m)$ is estimated for every class in a node
- How to estimate p_{mk} for class k and node R_m?

Class proportions

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

- For any node (leave), a label can be assigned

$$k(m) = \arg\max_k \hat{p}_{mk}$$

Classification trees

- Impurity measure $Q(R_m)$
  - R_m is a tree node (region)
  - Node can be split unless it is pure

Misclassification error: $\frac{1}{N_m}\sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}$

Gini index: $\sum_{k \neq k'} \hat{p}_{mk}\hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$

Cross-entropy or deviance: $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$.

- Note: In many sources, deviance is $Q(R_m)$ $N(R_m)$

Example: Cross –entropy is MLE of $Y_j|T \sim Multinomial(p_{j1}, \ldots p_{jc})$

Fitting regression trees: CART

Step 1: Finding optimal tree: grow the tree in order to minimize global objective

1. Let C_0 be a hypercube containing all observations
2. Let queue C={C_0}
3. Pick up some C_j from C and find a variable X_j and value s that split C_j into two hypercubes

$$R_1(j,s) = \{X|X_j \leq s\} \text{ and } R_2(j,s) = \{X|X_j > s\}$$

and solve

$$\min_{j,s}[N_1 Q(R_1) + N_2 Q(R_2)]$$

4. Remove C_j from C and add R_1 and R_2
5. Repeat 3-4 as many times as needed (or until each cube has only 1 observation)

CART: comments

- Greedy algorithm (optimal tree is not found)
- The largest tree will interpolate the data → large trees = overfitting the data
- Too small trees=underfitting (important structure may not be captured)
- Optimal tree length?

Optimal trees

- **Postpruning**

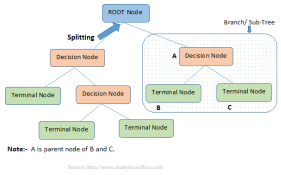
Weakest link pruning:

1. Merge two leaves that have smallest *N(parent)*Q(parent)-N(leave1)Q(leave1)-N(leave2)Q(leave2)*
2. For the current tree T, compute

$$I(T) = \sum_{R_i \in leaves} N(R_i)Q(R_i) + \alpha|T|$$

$|T|$ =#leaves

3. Repeat 1-2 until the tree with one leave is obtained
4. Select the tree with smallest I(T)



How to find the optimal α? Cross validation!

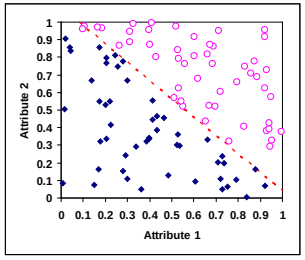
Decision trees: comments

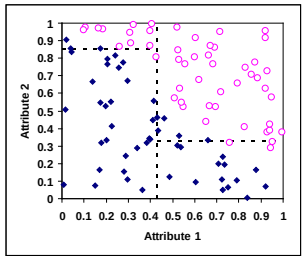
- Similar algorithms work for regression trees – replace $N \cdot Q(R)$ by $SSE(R)$
- Easy to interpret
- Easy to handle all types of features in one model
- **Automatic variable selection**
- Relatively robust to outliers
- Handle large datasets

- Trees have high variance: a small change in response→ totally different tree
- Greedy algorithms → fit may be not so good
- Lack of smoothness

Decision trees: issues

- Large trees may be needed to model an easy system:





Decision trees in R

- **tree** package
  - Alternative: **rpart**

tree(formula, data, weights, control, split = c("deviance", "gini"), …)

print(), summary(), plot(), text()

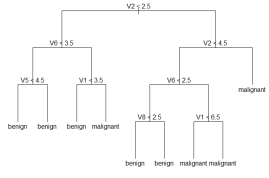
Example: breast cancer as a function av biological measurements

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


Decision trees in R

- Adjust the splitting in the tree with *control* parameter (leaf size for ex)

```
> fit
node), split, n, deviance, yval, (yprob)
      * denotes terminal node

 1) root 683 884.400 benign ( 0.650073 0.349927 )
   2) V2 < 2.5 418 108.900 benign ( 0.971292 0.028708 )
     4) V6 < 3.5 395  25.130 benign ( 0.994937 0.005063 )
       8) V5 < 4.5 389   0.000 benign ( 1.000000 0.000000 ) *
       9) V5 > 4.5 6   7.638 benign ( 0.666667 0.333333 ) *
     5) V6 > 3.5 23  31.490 benign ( 0.565217 0.434783 )
      10) V1 < 3.5 11   0.000 benign ( 1.000000 0.000000 ) *
      11) V1 > 3.5 12  10.810 malignant ( 0.166667 0.833333 ) *
   3) V2 > 2.5 265 217.900 malignant ( 0.143396 0.856604 )
     6) V2 < 4.5 90 120.300 malignant ( 0.388889 0.611111 )
      12) V6 < 2.5 30  27.030 benign ( 0.833333 0.166667 )
        24) V8 < 2.5 19   0.000 benign ( 1.000000 0.000000 ) *
        25) V8 > 2.5 11  15.160 benign ( 0.545455 0.454545 ) *
      13) V6 > 2.5 60  54.070 malignant ( 0.166667 0.833333 )
        26) V1 < 6.5 28  35.160 malignant ( 0.321429 0.678571 ) *
        27) V1 > 6.5 32   8.900 malignant ( 0.031250 0.968750 ) *
     7) V2 > 4.5 175  30.350 malignant ( 0.017143 0.982857 ) *
```




```
> summary(fit)

Classification tree:
tree(formula = class ~ ., data = biopsy)
Variables actually used in tree construction:
[1] "V2" "V6" "V5" "V1" "V8"
Number of terminal nodes:  9
Residual mean deviance:  0.1603 = 108 / 674
Misclassification error rate: 0.03221 = 22 / 683
```

Decision trees in R

- Misclassification results

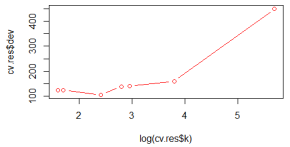
```
Yfit=predict(fit, newdata=biopsy, type="class")
table(biopsy$class,Yfit)
```

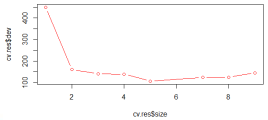
```
> table(biopsy$class,Yfit)
           Yfit
            benign malignant
  benign       440        18
  malignant      7       234
```


Decision trees in R

- Selecting optimal tree by penalizing
  - 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")
```



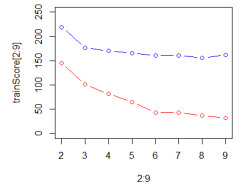


What is optimal number of leaves?

Decision trees in R

- 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")
```



What is optimal number of leaves?

Decision trees in R

- Final tree: 5 leaves

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

```
> table(valid$class,Yfit)
           Yfit
            benign malignant
  benign       222         8
  malignant      6       114
```

Generalized Linear Models. Uncertainty estimation

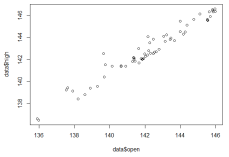
Lecture 2c

Moving beyond typical distributions

- We know how to model
  - Normally distributed targets -> linear regression
  - Bernoulli and Multinomial targets→logistic regression
  - What if target distribution is more complex?

Example 1: Daily Stock prices NASDAQ
- Open
- High (within day)

Does it seem that the error is normal here?



Example 2: Number of calls to bank
- Y=Number of calls
- X= time

Endless amount of classes → multinomial does not work… (Poisson)

Exponential family

- More advanced error distributions are sometimes needed!
- Many distributions belong to **exponential** family:
  - Normal, Exponential, Gamma, Beta, Chi-squared..
  - Bernoulli, Multinoulli, Poisson…

$$p(\boldsymbol{x}|\boldsymbol{\eta}) = h(\boldsymbol{x})g(\boldsymbol{\eta})e^{(\boldsymbol{\eta}^T u(\boldsymbol{x}))}$$

- Easy to find MLE and MAP
- Non-exponential family distributions: uniform, Student t

Example: Bernoulli

Generalized linear models

- Assume Y from the exponential family
- **Model** is $Y \sim EF(\mu, \dots),\ f(\mu) = \boldsymbol{w}^T\boldsymbol{x}$
  - Alt $\mu = f^{-1}(\boldsymbol{w}^T\boldsymbol{x})$
  - f^{-1} is activation function
  - f is link function (in principle, arbitrary)
- Arbitrary f will lead to (s – dispersion parameter)

$$p(y|w,s) = h(y,s)g(\boldsymbol{w},\boldsymbol{x})e^{\frac{b(\boldsymbol{w},\boldsymbol{x})y}{s}}$$

- If f is a canonical link, then

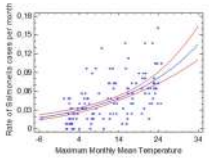
$$p(y|w,s) = h(y,s)g(\boldsymbol{w},\boldsymbol{x})e^{\frac{(\boldsymbol{w}^T\boldsymbol{x})y}{s}}$$

Generalized linear models

- Canonical links are normally used
  - MLE computations simplify
  - MLE $\hat{w} = F(X^TY)$ → computations do not depend on all data but rather a summary (sufficient statistics)→ computations speed up

Example: Poisson regression

$f^{-1}(\mu) = e^{\mu}, Y \sim Poisson\left(e^{\boldsymbol{w}^T\boldsymbol{x}}\right)$

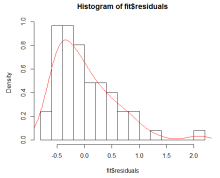


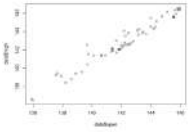
Generalized linear model: software

- Use **glm**(formula, family, data) in R

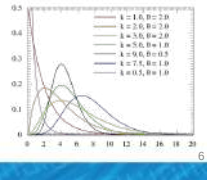
Example: Daily Stock prices NASDAQ
- Open
- High (within day)

1. Try to fit usual linear regression, study histogram of residuals



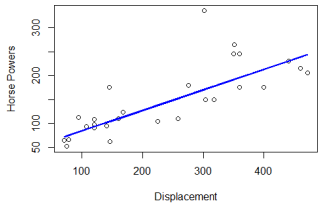


Gamma distribution: Wikipedia



Least absolute deviation regression

- Model $Y \sim Laplace(w^TX, b)$
  - Member of exponential family
- Equivalent to minimizing sum of absolute deviations
- Properties
  - Robust to outliers
  - Sensitive to changes in data
  - Multiple solutions possible



- R: package **L1pack**

Probabilistic models

- Why it is beneficial to assume a **probabilistic** model?
- A common approach to modelling in CS and engineering:

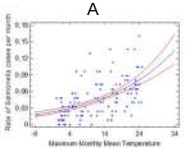
$$y = f(x, w)$$

- f is known, w is unknown
- Fit model to data with least squares, optimization or ad hoc→ find w

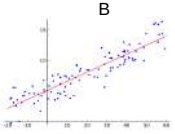
Probabilistic models

Arguments against deterministic models:
- The model does not really describe actual data (error is not explained)
  - No difference between modelling data A (Poisson) and B (Normal)
  - Estimation strategy for A is not good for B
- The model typically gives a **deterministic answer**, no information about uncertainty
  - "…The exchange rate tomorrow will be 8.22 …" 😨

A



B



Probabilistic models

Probabilistic model

$$Y \sim Distribution(f(x,w),\theta)$$

- Data is fully explained (error as well)
- Automatic principle for finding parameters: MLE , MAP or Bayes theorem
- Automatic principle for finding uncertainty (conf. limits)
  - **Bootstrap**
  - Posterior probability
- Possibility to generate new data of the same type
  - Further testing of the model

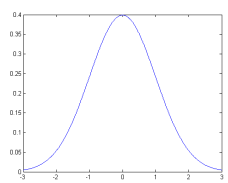
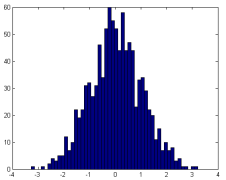
Uncertainty estimation

- Given estimator $\hat{f} = \hat{f}(x, D)$ (or $\hat{\boldsymbol{\alpha}} = \delta(D)$), how to estimate the uncertainty?

- Answer 1: if the distribution for data *D* is given, compute analytically the distribution for the estimator→ derive confidence limits
  - Often difficult
  - Example: In simple linear regression, $\hat{\alpha}$ follows *t* distribution

- Answer 2: Use **bootstrap**

The bootstrap: general principle

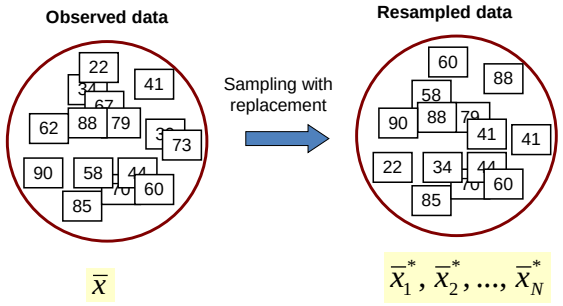



We want to determine uncertainty of $\hat{f}(D, X)$

1. Generate many different D_i from their distribution
2. Use histogram of $\hat{f}(D_i, X)$ to determine confidence limits→ unfortunately can not be done (distr of *D is often unknown)*

Instead: Generate many different D_i^* from the empirical distribution (histogram)

Nonparametric bootstrap



$\bar{x}$ $\quad \bar{x}_1^*, \bar{x}_2^*, \ldots, \bar{x}_N^*$

Nonparametric bootstrap

Given estimator $\hat{w} = \hat{f}(D)$

Assume $X \sim F(X, w)$, F and w are unknown

1. Estimate $\hat{w}$ from data **D**=(X_1,…X_n)
2. Generate $\mathbf{D_1}$ =(X^*_1,…X^*_n) by sampling with replacement
3. Repeat step 2 B times
4. The distribution of w is given by $\hat{f}(D_1)$, … $\hat{f}(D_B)$

Nonparametric bootstrap can be applied to any deterministic estimator, distribution-free

Parametric bootstrap

Given estimator $\hat{w} = \hat{f}(D)$

Assume $X \sim F(X, w)$, F is known and w is unknown

1. Estimate $\hat{w}$ from data **D**=(X_1,…X_n)
2. Generate $\mathbf{D_1}$ =(X^*_1,…X^*_n) by generating from $F(X, \hat{w})$
3. Repeat step 2 B times
4. The distribution of w is given by $\hat{f}(D_1)$, … $\hat{f}(D_B)$

Parametric bootstrap is **more** precise if the distribution form is correct

Uncertainty estimation

1. Get D_1 , … D_B by bootstrap
2. Use $\hat{f}(D_1)$, … $\hat{f}(D_B)$ to estimate the uncertainty
   - Boostrap percentile
   - Bootstrap Bca
   - …

- Bootstrap works for all distribution types
- Can be bad accuracy for small data sets $n < 40$ (empirical is far from true)
- Parametric bootstrap works even for small samples

Bootstrap confidence intervals

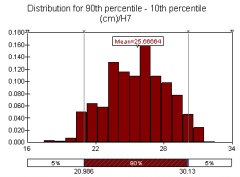
- To estimate 100(1-α) confidence interval for w

Bootstrap percentile method

1. Using bootstrap, compute $\hat{f}(D_1)$, … $\hat{f}(D_B)$, sort in ascending order, get w_1 … w_B
2. Define A_1=ceil(B α/2), A_2=floor(B-B α/2)
3. Confidence interval is given by

$$\left(w_{A_1}, w_{A_2}\right)$$

Look at the plot…



Bootstrap: regression context

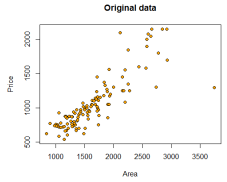
- Model $Y \sim F(X, w)$
- Data $\mathrm{D} = \{(Y_i, X_i), i = 1, \ldots, n\}$
- Idea: produce several bootstrap sets that are similar to D

Nonparametric bootstrap:

1. Using observation set **D**, sample **pairs** (X_i, Y_i) with replacement and get bootstrap sample $\mathbf{D_1}$
2. Repeat step 1 B times→ get $\mathbf{D_{1,\ldots}}$ $\mathbf{D_B}$

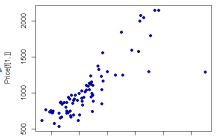
Uncertainty estimation

Example: Albuquerque dataset:
Y=Price of House
X=Area (sqft)

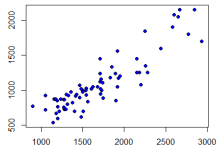


We sample data index, from {1…N}

D_1



D_{50}



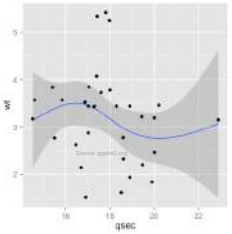
Bootstrap: regression context

Parametric bootstrap

1. Fit a model to D → get $\hat{w}(D)$.
2. Set $X_i^* = X_i$, generate $Y_i^* \sim F(X_i, \hat{w})$.
3. $D_i = \{(X_i^*, Y_i^*), i = 1, \dots, n\}$
4. Repeat step 2 B times

Confindence intervals in regression

- Given $Y \sim Distribution(y|x,w), EY|X = \mu|x = f(x,w)$
  - Example: $Y \sim N(w^T x, \sigma^2), \mu|x = f(x,w) = w^T x$
- Estimate intervals for $\mu|x = f(x,w)$ for many X, combine in a **confidence band**
- What is estimator?
  - $\mu|x = f(x,w)$



Confindence intervals in regression

Estimation

1. Compute $D_1, \dots D_B$ using a bootstrap
2. Fit model to $D_1, \dots D_B$ →estimate $\hat{W}_1, \dots \hat{W}_B$
3. For a given X, compute $f(X, \hat{w}_1), \dots f(X, \hat{w}_B)$ and estimate confidence interval by (percentile method)
4. Combine confidence intervals in a band

Bootstrap: R

- Package **boot**
  - **Functions:**
    - boot()
    - boot.ci() – 1 parameter
    - envelope() – many parameters
- Random random generation for parametic bootstrap:
  - Rnorm()
  - Runif()
  - …

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

Bootstrap: R

Nonparametric bootstrap:

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

```
library(boot)
data2=data[order(data$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
```


Bootstrap: R

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 *statistic* that depend on *data* which will be generated by *ran.gen* and should return the estimator

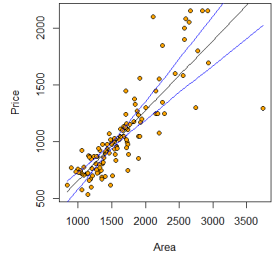
Bootstrap

```
mle=lm(Price~Area, data=data2)

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(mle$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")
```


Uncertainty estimation: R

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



Prediction bands

- Confidence interval for Y|X= interval for mean $EY|X$
- Prediction interval for Y|X= interval for $Y|X$

$$Y \sim Distribution(x, w)$$

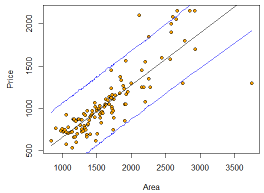
Prediction band for parametric bootstrap

1. Run parametric bootstrap and get $D_1, \dots D_B$
2. Fit the model to the data and get $\hat{w}(D_1), \dots \hat{w}(D_B)$
3. For each X, generate from $Distribution\left(X, \hat{w}(D_1)\right), \dots$ $Distribution\left(X, \hat{w}(D_B)\right)$ and apply percentile method
4. Connect the intervals→get the band

Estimation of the model quality

Example: parametric bootstrap

```
mle=lm(Price~Area, data=data2)

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)
  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")
```



Why wider band?

Lecture 2d

Latent variable models

Overview

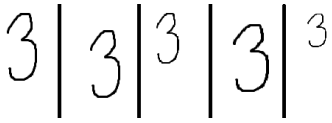
- Principal Component Analysis (PCA)
- Probabilistic PCA
- Independent component analysis (ICA)

Latent variables

- Sometimes data depends on the variables we can not measure (hard to measure)
  - Answers on the test depend on Intelligence
  - Brain activity in the brain is measured by sensors
  - Stock prices depend on market confidence

Latent variables

- Latent factor discovered→ data storage may decrease a lot
- Latent factors
  - Center
  - Scaling
- Original vs compressed
  - 100x100x5=50000
  - 100x100+2*5+2*5=10020



Principal Component Analysis (PCA)

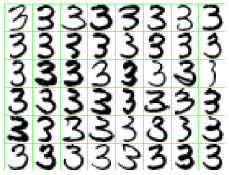
- *PCA* is a technique for reducing the complexity of high dimensional data
- It can be used to approximate high dimensional data with a few dimensions (latent features) –> much less data to store
- New variables might have a special interpretation

Applications

- Image recognition
- Information compression
- Subspace clustering
- …

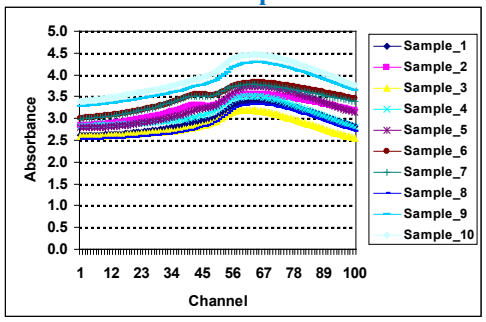
Principal Component Analysis (PCA)

- Example 1: Hadwritten digits
  - Can we get a more compact summary?



Absorbance records for ten samples of chopped meat

Parallel coordinate plot for "FAT"



1 target (fat)

100 features (absorbance at 100 wavelengths or channels)

The features are strongly correlated to each other

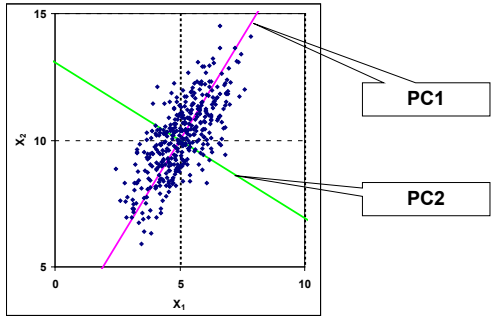
Principal components analysis

Idea: Introduce a new coordinate system (PC1, PC2, …) where

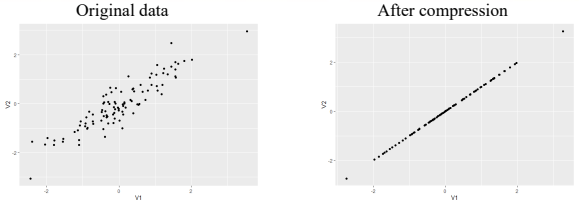
- The first principal component (PC1) is the direction that maximizes the variance of the projected data
- The second principal component (PC2) is the direction that maximizes the variance of the projected data after the variation along PC1 has been removed
- The third principal component (PC3) is the direction that maximizes the variance of the projected data after the variation along PC1 and PC2 has been removed
- ….

In the new coordinate system, coordinates corresponding to the last principal components are very small → can take away these columns

Principal Component Analysis - two inputs



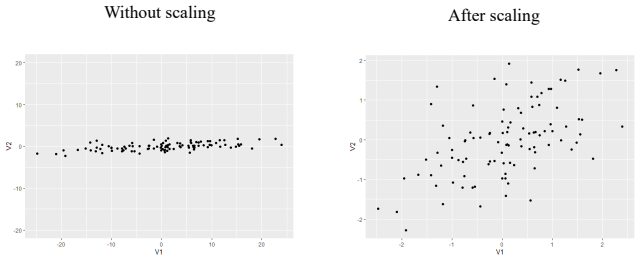
PCA- after reducing dimensionality



- Data became approximate (but less data to store)
- $PC_1, \dots PC_M$ are actually eigenvections of **sample covariance** (first largest eigenvalue,…,Mth largest egenvalue)

PCA and scaling

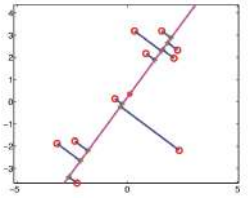
- Do we need to scale features?



PCA: another view

- Aim: minimize the distance between the original and projected data

$$\min_{U_M} \sum_{i=1}^{N} \|x_n - \tilde{x}_n\|^2$$



PCA: computations

Data $D = \left\| \mathbf{x}_1 \ \mathbf{x}_2 \ \dots \mathbf{x}_p \right\|, \quad \mathbf{x}_i = (x_{i1}, \dots, x_{in})$

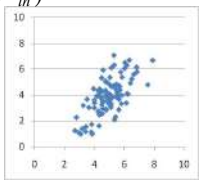
1. Centred data

$$X = \left\| \mathbf{x}_1 - \overline{\mathbf{x}}_1 \ \mathbf{x}_2 - \overline{\mathbf{x}}_2 \ \dots \mathbf{x}_p - \overline{\mathbf{x}}_p \right\|,$$

2. Covariance matrix

$$\boldsymbol{S} = \frac{1}{N} \boldsymbol{X}^T \boldsymbol{X}$$

3. Search for eigenvectors and eigenvalues of **S**



	Column 1	Column 2
Column 1	0.951	0.905
Column 2	0.905	1.883

PCA: computations

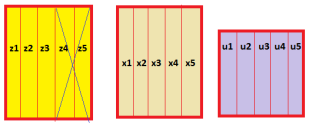
4. Coordinates of any data point x=(x_1…x_p) in the new coordinate system:
$z = (z_1, \dots z_n),\ z_i = x^T u_i$

Matrix form: $Z = X\ U$

5. Discard principle components after some *M:*
$Z = X\ U_M$

6. New data will have dimensions N x M instead of N x p

Getting approximate original data:
$\tilde{X} = Z U_M^T$

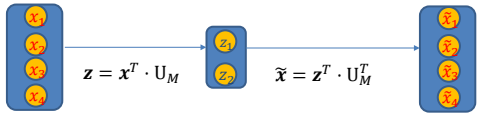


Store: N x M+ p x M instead N x p

100*50 vs
100*4+50*4

PCA: computations

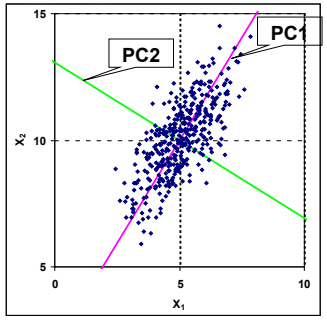
- PCA makes a **linear** compression of features



R^p $\quad R^M, M < p \quad$ R^p

$$\min_{U_M} \sum_{i=1}^{N} \|x_n - \tilde{x}_n\|^2$$

Principal Component Analysis



Eigenanalysis of the Covariance Matrix

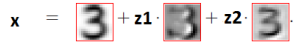
Eigenvalue	2.8162	0.3835
Proportion	0.880	0.120
Cumulative	0.880	1.000

Variable	PC1	PC2
X1	0.523	0.852
X2	0.852	-0.523

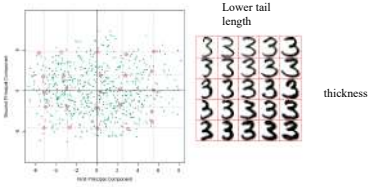
Loadings (U)

Principal Component Analysis

- Digits: two eigenvectors extracted



- Interptretation of eigenvectiors

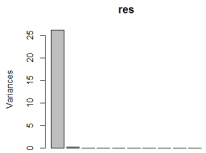


PCA in R

- Prcomp(), biplot(), screeplot()

```
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)
```

```
> lambda
  [1] 2.612713e+01 2.385369e-01 7.844883e-02 3.018501e-
  [7] 2.052212e-04 1.084213e-04 2.077326e-05 1.150359e-

> sprintf("%2.3f",lambda/sum(lambda)*100)
  [1] "98.679" "0.901"  "0.296"  "0.114"  "0.006
  [9] "0.000"  "0.000"  "0.000"  "0.000"  "0.000
```



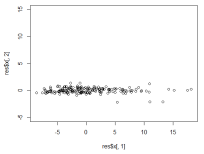
Only 1 component captures the 99% of variation!

PCA in R

- Principal component **loadings (U)**

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

```
> head(U)
              PC1         PC2         PC3
Channel1 0.07938192 0.1156228 0.08073156 -0.0927
Channel2 0.07987445 0.1170972 0.07887873 -0.0981
Channel3 0.08036498 0.1185571 0.07702127 -0.1031
Channel4 0.08085611 0.1200006 0.07515015 -0.1077
Channel5 0.08135022 0.1214075 0.07323819 -0.1119
Channel6 0.08184806 0.1227491 0.07125048 -0.1156
```



- Data in (PC1, PC2) – **scores (Z)**

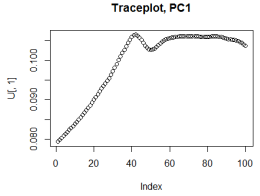
```
plot(res$x[,1], res$x[,2], ylim=c(-5,15))
```

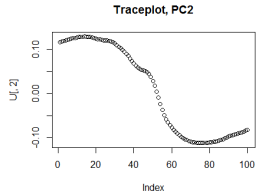
Do we need second dimension?

PCA in R

- Trace plots

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

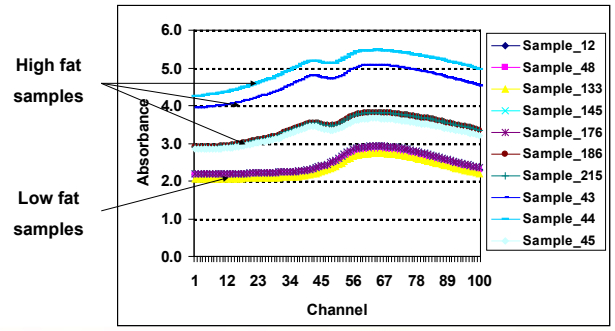




Which components contribute to PC1-2?

Absorbance records for ten samples of chopped meat

PCA2 captures the most of remaining variation



Probabilistic PCA

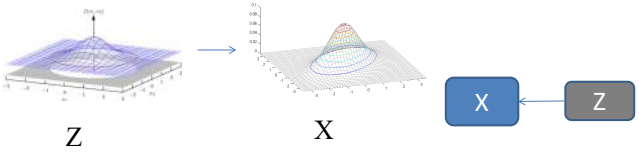
- z_i-latent variables, x_i- observed variables

$$\boldsymbol{z}\sim\boldsymbol{N}(0,\boldsymbol{I})$$
$$\boldsymbol{x}|\boldsymbol{z}\sim\boldsymbol{N}(\boldsymbol{x}|\boldsymbol{Wz}+\boldsymbol{\mu},\sigma^2\boldsymbol{I})$$

- Alternatively

$$\boldsymbol{z}\sim\boldsymbol{N}(0,\boldsymbol{I}),\boldsymbol{x}=\boldsymbol{\mu}+\boldsymbol{Wz}+\boldsymbol{\epsilon},\boldsymbol{\epsilon}\sim\boldsymbol{N}(\boldsymbol{0},\boldsymbol{\sigma^2 I})$$

- **Interpretation**: Observed data (X) is obtained by rotation, scaling and translation of standard normal distribution (Z) and adding some noise.



Probabilistic PCA

- **Aim**: extract Z from X
- Distribution of x:

$$\boldsymbol{x}\sim\boldsymbol{N}(\boldsymbol{\mu},\boldsymbol{C})$$
$$\boldsymbol{C}=\boldsymbol{WW^T}+\boldsymbol{\sigma^2 I}$$

- Rotation invariance
  - Assume that x was generated from $z'=Rz, RR^T=I,\ p(x)$ does not change!

$$\boldsymbol{x}|\boldsymbol{z'}\sim\boldsymbol{N}(\boldsymbol{x}|\boldsymbol{Wz'}+\boldsymbol{\mu},\sigma^2\boldsymbol{I})$$

  - **Model will not be able find latent factors uniquely!** ☹
    - It does not distinguish z from z'

Probabilistic PCA

- Estimation of parameters: ML

Theorem. ML estimates are given by

$$\mu_{ML}=\bar{x}$$
$$W_{ML}=U_M(L_M-\sigma_{ML}^2 I)^{\frac{1}{2}}R$$
$$\sigma_{ML}^2=\frac{1}{p-M}\sum_{i=M+1}^{p}\lambda_i$$

- U_M matrix of M eigenvectors
- L_M diagonal matrix of M eigenvalues
- R any orthogonal matrix

Probabilistic PCA

- Estimation of Z
  - Use mean of posterior

$$\hat{z}=(W_{ML}^T W_{ML}+\sigma_{ML}^2 I)^{-1}W_{ML}^T(x-\mu)$$

- Connection to standard PCA
  - Assume $R=I,\sigma^2=0$→get standard PCA components scaled by inverse root of eigenvalues

$$Z=XUL^{-\frac{1}{2}}$$

Advantages of probabilistic PCA

- More settings to specify→ more flexible
- Can be faster when M<<p
- Missing values can be handled
- M can be derived if a Bayesian version is used
- Probabilistic PCA can be applied to classification problems directly
- Probabilistic PCA can generate new data

Probabilistic PCA in R

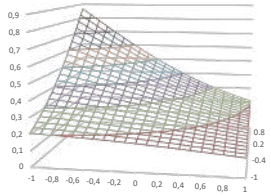
- Use **pcaMethods** from Bioconductor
- Install
  - source("https://bioconductor.org/biocLite.R")
  - biocLite("pcaMethods")

Ppca(data, nPcs,…)

Results: scores, loadings…

Independent component analysis (ICA)

- Probabilistic PCA does not capture latent factors
  - Rotation invariance
- Let's choose distribution which is not rotation invariant→will get unique latent factors
- Choose non-Gaussian $p(z_i)$
- Assuming latent features are **independent**



$$p(z) = \prod_{i=1}^{M} p(z_i) \qquad p(z_i) = \frac{2}{\pi(e^{z_i} + e^{-z_i})}$$

ICA

- Model

$$x = \mu + Wz + \epsilon, \qquad \epsilon \sim \boldsymbol{N}(0, \Sigma)$$

- **Estimation : Maximum likelihood** ($V = W^{-1}$)
  - Assuming noise-free x

$$\max_{V} \sum_{i=1}^{n} \sum_{j=1}^{p} \log\left(p_j(v_j^T x_i)\right)$$

Subject to $||v_i|| = 1$

ICA: estimation algorithm

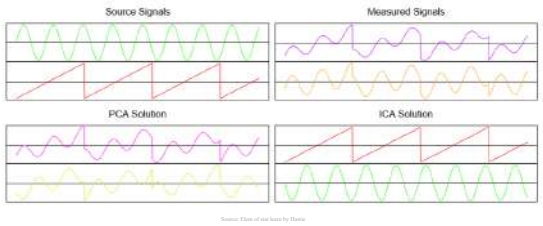
1. Estimate V by maximum likelihood
2. Compute $Z = X'V$

- **With prewhitening**
  1. Convert X into PCA coordinate system (do not remove dimensions): $X' = XU$
  2. Estimate V by maximum likelihood in ICA
  3. Estimate final scores $Z = X'V$

  – Note: full transformation matrix is $U_{ICA} = U \cdot V$

ICA

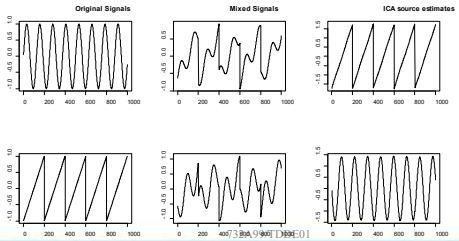
- Example



Independent component analysis: R

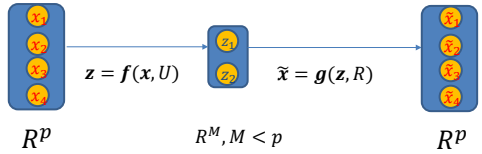
R package: fastICA

```
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
```



Autoencoders (nonlinear PCA)

- Why linear transformations? Take nonlinear instead!
- $f()$ and $g()$ are typically Neural Networks



$\boldsymbol{z} = \boldsymbol{f}(\boldsymbol{x}, U)$ $\quad \tilde{\boldsymbol{x}} = \boldsymbol{g}(\boldsymbol{z}, R)$

R^p $\quad R^M, M < p$ $\quad R^p$

$$\min_{U,R} \sum_{i=1}^{N} \|x_n - \tilde{x}_n\|^2$$

…or some other loss function

Histogram Classification

- Consider binary classification with input space $\mathbb{R}^D$.
- The best classifier under the 0-1 loss function is $y^*(\boldsymbol{x}) = \arg\max_y p(y|\boldsymbol{x})$.
- Since $\boldsymbol{x}$ may not appear in the finite training set $\{(\boldsymbol{x}_n, t_n)\}$ available, then
  - divide the input space into D-dimensional cubes of side h, and
  - classify according to majority vote in the cube $C(\boldsymbol{x}, h)$ that contains $\boldsymbol{x}$.

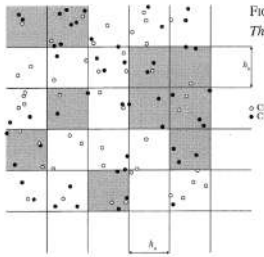


FIGURE 6.1. *A cubic histogram rule: The decision is 1 in the shaded area.*

- In other words,

$$y_C(\boldsymbol{x}) = \begin{cases} 0 & \text{if } \sum_n \mathbf{1}_{\{t_n=1, \boldsymbol{x}_n \in C(\boldsymbol{x},h)\}} \leq \sum_n \mathbf{1}_{\{t_n=0, \boldsymbol{x}_n \in C(\boldsymbol{x},h)\}} \\ 1 & \text{otherwise} \end{cases}$$

Moving Window Classification

- The histogram rule is less accurate at the borders of the cube, because those points are not as well represented by the cube as the ones near the center. Then,
  - consider the points within a certain distance to the point to classify, and
  - classify the point according to majority vote.

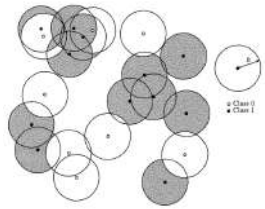


FIGURE 10.1. *The moving window rule in $\mathbb{R}^2$. The decision is 1 in the shaded area.*

- In other words,

$$y_S(\boldsymbol{x}) = \begin{cases} 0 & \text{if } \sum_n \mathbf{1}_{\{t_n=1, \boldsymbol{x}_n \in S(\boldsymbol{x},h)\}} \leq \sum_n \mathbf{1}_{\{t_n=0, \boldsymbol{x}_n \in S(\boldsymbol{x},h)\}} \\ 1 & \text{otherwise} \end{cases}$$

where $S(\boldsymbol{x}, h)$ is a D-dimensional closed ball of radius h centered at $\boldsymbol{x}$.

Kernel Classification

- The moving window rule gives equal weight to all the points in the ball, which may be counterintuitive. Then,

$$y_k(\boldsymbol{x}) = \begin{cases} 0 & \text{if } \sum_n \mathbf{1}_{\{t_n=1\}} k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right) \leq \sum_n \mathbf{1}_{\{t_n=0\}} k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right) \\ 1 & \text{otherwise} \end{cases}$$

where $k : \mathbb{R}^D \to \mathbb{R}$ is a kernel function, which is usually non-negative and monotone decreasing along rays starting from the origin. The parameter h is called smoothing factor or width.

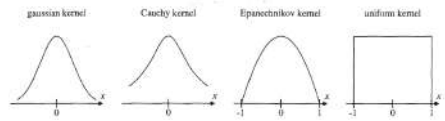


FIGURE 10.3. *Various kernels on $\mathcal{R}$.*

- Gaussian kernel: $k(u) = exp(-\|u\|^2)$ where $\|\cdot\|$ is the Euclidean norm.
- Cauchy kernel: $k(u) = 1/(1 + \|u\|^{D+1})$
- Epanechnikov kernel: $k(u) = (1 - \|u\|^2)\mathbf{1}_{\{\|u\| \leq 1\}}$
- Moving window kernel: $k(u) = \mathbf{1}_{\{u \in S(0,1)\}}$

Kernel Classification

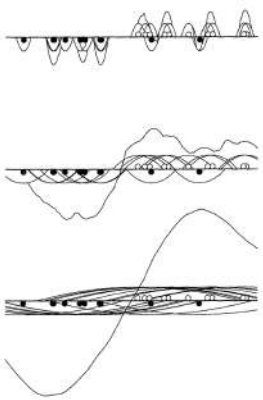


FIGURE 10.2. *Kernel rule on the real line. The figure shows $\sum_{i=1}^n (2Y_i - 1)K((x - X_i)/h)$ for $n = 20$, $K(u) = (1 - u^2)I_{[|u| \leq 1]}$ (the Epanechnikov kernel), and three smoothing factors h. One definitely undersmooths and one oversmooths. We took $p = 1/2$, and the class-conditional densities are $f_0(x) = 2(1 - x)$ and $f_1(x) = 2x$ on $[0, 1]$.*

Histogram, Moving Window, and Kernel Regression

- Consider regressing an unidimensional continuous random variable on a D-dimensional continuous random variable.
- The best regression function under the squared error loss function is $y^*(\boldsymbol{x}) = \mathbb{E}_Y[y|\boldsymbol{x}]$.
- Since $\boldsymbol{x}$ may not appear in the finite training set $\{(\boldsymbol{x}_n, t_n)\}$ available, then we average over the points in $C(\boldsymbol{x}, h)$ or $S(\boldsymbol{x}, h)$, or kernel-weighted average over all the points.
- In other words,

$$y_C(\boldsymbol{x}) = \frac{\sum_{\boldsymbol{x}_n \in C(\boldsymbol{x},h)} t_n}{|\{\boldsymbol{x}_n \in C(\boldsymbol{x}, h)\}|}$$

or

$$y_S(\boldsymbol{x}) = \frac{\sum_{\boldsymbol{x}_n \in S(\boldsymbol{x},h)} t_n}{|\{\boldsymbol{x}_n \in S(\boldsymbol{x}, h)\}|}$$

or

$$y_k(\boldsymbol{x}) = \frac{\sum_n k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right) t_n}{\sum_n k\left(\frac{\boldsymbol{x}-\boldsymbol{x}_n}{h}\right)}$$

Histogram, Moving Window, and Kernel Density Estimation

- Consider density estimation for a D-dimensional continuous random variable.
- Let $R \subseteq \mathbb{R}^D$ and $\boldsymbol{x} \in R$. Then,

$$P = \int_R p(\boldsymbol{x}) d\boldsymbol{x} \simeq p(\boldsymbol{x}) Volume(R)$$

and the number of the N training points $\{\boldsymbol{x}_n\}$ that fall inside R is

$$|\{\boldsymbol{x}_n \in R\}| \simeq P\, N$$

and thus

$$p(\boldsymbol{x}) \simeq \frac{|\{\boldsymbol{x}_n \in R\}|}{N\, Volume(R)}$$

- Then,

$$p_C(\boldsymbol{x}) = \frac{|\{\boldsymbol{x}_n \in C(\boldsymbol{x}, h)\}|}{N\, Volume(C(\boldsymbol{x}, h))}$$

or

$$p_S(\boldsymbol{x}) = \frac{|\{\boldsymbol{x}_n \in S(\boldsymbol{x}, h)\}|}{N\, Volume(S(\boldsymbol{x}, h))}$$

or

$$p_k(\boldsymbol{x}) = \frac{1}{N} \sum_n k\left(\frac{\boldsymbol{x} - \boldsymbol{x}_n}{h}\right)$$

assuming that $k(u) \geq 0$ for all u and $\int k(u) du = 1$.

Histogram, Moving Window, and Kernel Density Estimation

Figure 2.24 An illustration of the histogram approach to density estimation, in which a data set of 50 data points is generated from the distribution shown by the green curve. Histogram density estimates, based on (2.241), with a common bin width Δ are shown for various values of Δ.

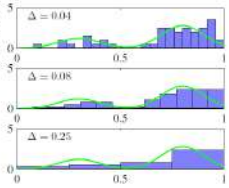
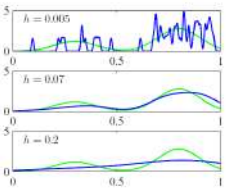


Figure 2.25 Illustration of the kernel density model (2.250) applied to the same data set used to demonstrate the histogram approach in Figure 2.24. We see that h acts as a smoothing parameter and that if it is set too small (top panel), the result is a very noisy density model, whereas if it is set too large (bottom panel), then the bimodal nature of the underlying distribution from which the data is generated (shown by the green curve) is washed out. The best density model is obtained for some intermediate value of h (middle panel).



Histogram, Moving Window, and Kernel Density Estimation

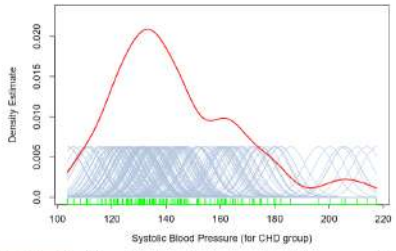


FIGURE 6.13. *A kernel density estimate for systolic blood pressure (for the CHD group). The density estimate at each point is the average contribution from each of the kernels at that point. We have scaled the kernels down by a factor of 10 to make the graph readable.*

Histogram, Moving Window, and Kernel Density Estimation

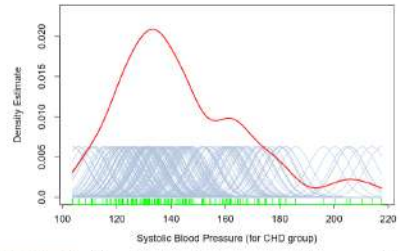


FIGURE 6.13. *A kernel density estimate for systolic blood pressure (for the CHD group). The density estimate at each point is the average contribution from each of the kernels at that point. We have scaled the kernels down by a factor of 10 to make the graph readable.*

- From kernel density estimation to kernel classification:
  1. Estimate $p(\boldsymbol{x}|y = 0)$ and $p(\boldsymbol{x}|y = 1)$ using the methods just seen.
  2. Estimate $p(y)$ as class proportions.
  3. Compute $p(y|\boldsymbol{x}) \propto p(\boldsymbol{x}|y)p(y)$ by Bayes theorem.

Histogram, Moving Window, and Kernel Density Estimation

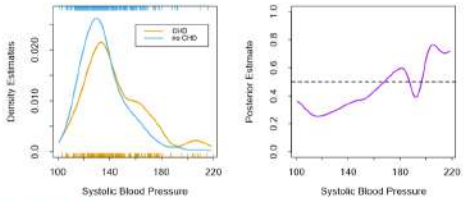
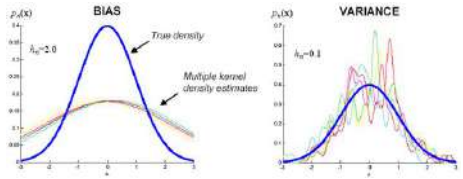


FIGURE 6.14. *The left panel shows the two separate density estimates for systolic blood pressure in the CHD versus no-CHD groups, using a Gaussian kernel density estimate in each. The right panel shows the estimated posterior probabilities for CHD, using (6.25).*

Kernel Selection

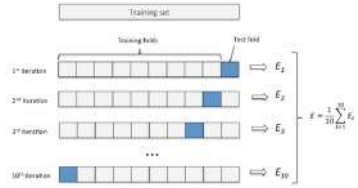
- How to choose the right kernel and width ? E.g., by cross-validation.
- What does "right" mean ? E.g., minimize loss function.
- Note that the width of the kernel corresponds to a bias-variance trade-off.



- Small width implies considering few points. So, the variance will be large (similar to the variance of a single point). The bias will be small since the points considered are close to $\boldsymbol{x}$.
- Large width implies considering many points. So, the variance will be small and the bias will be large.

Kernel Selection

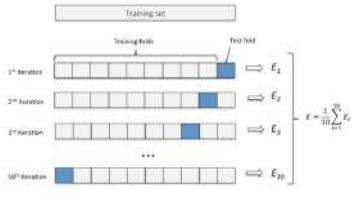
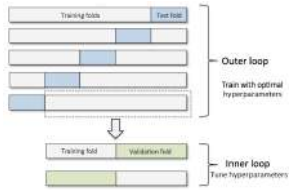
- Recall the following from previous lectures.
- Cross-validation is a technique to estimate the prediction error of a model.



- If the training set contains N points, note that cross-validation estimates the prediction error when the model is trained on $N - N/K$ points.
- Note that the model returned is trained on N points. So, cross-validation overestimates the prediction error of the model returned.
- This seems to suggest that a large K should be preferred. However, this typically implies a large variance of the error estimate, since there are only N/K test points.
- Typically, $K = 5, 10$ works well.

Kernel Selection

- Model: For example, ridge regression with a given value for the penalty factor λ. Only the parameters (weights) need to be determined (closed-form solution).
- Model selection: For example, determine the value for the penalty factor λ. Another example, determine the kernel and width for kernel classification, regression or density estimation. In either case, we do not have a continuous criterion to optimize. Solution: **Nested** cross-validation.

Cross-validation for estimating model prediction error	**Nested** cross-validation for estimating model **selection** prediction error
	

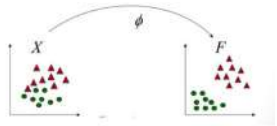
- Error overestimation may not be a concern for model selection. So, $K = 2$ may suffice in the inner loop.
- Which is the fitted model returned by nested cross-validation ?

Kernel Trick

- The kernel function $k\left(\frac{\boldsymbol{x}-\boldsymbol{x}'}{h}\right)$ is invariant to translations, and it can be generalized as $k(\boldsymbol{x}, \boldsymbol{x}')$. For instance,
  - Polynomial kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T\boldsymbol{x}' + c)^M$
  - Gaussian kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = exp(-\|\boldsymbol{x} - \boldsymbol{x}'\|^2/2\sigma^2)$
- If the matrix

$$\begin{pmatrix} k(\boldsymbol{x}_1, \boldsymbol{x}_1) & \dots & k(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ \vdots & \dots & \vdots \\ k(\boldsymbol{x}_N, \boldsymbol{x}_1) & \dots & k(\boldsymbol{x}_N, \boldsymbol{x}_N) \end{pmatrix}$$

is symmetric and positive semi-definite for all choices of $\{\boldsymbol{x}_n\}$, then $k(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T\phi(\boldsymbol{x}')$ where $\phi(\cdot)$ is a mapping from the input space to the feature space.



- The feature space may be non-linear and even infinite dimensional. For instance,

$$\phi(\boldsymbol{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c)$$

for the polynomial kernel with $M = D = 2$.

Kernel Trick

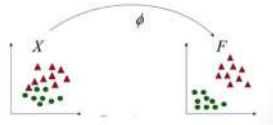
- Consider again moving window classification, regression, and density estimation.
- Note that $\boldsymbol{x}_n \in S(\boldsymbol{x}, h)$ if and only if $\|\boldsymbol{x} - \boldsymbol{x}_n\| \leq h$.
- Note that

$$\|\boldsymbol{x} - \boldsymbol{x}_n\| = \sqrt{(\boldsymbol{x} - \boldsymbol{x}_n)^T(\boldsymbol{x} - \boldsymbol{x}_n)} = \sqrt{\boldsymbol{x}^T\boldsymbol{x} + \boldsymbol{x}_n^T\boldsymbol{x}_n - 2\boldsymbol{x}^T\boldsymbol{x}_n}$$

- Then,

$$\begin{aligned} \|\phi(\boldsymbol{x}) - \phi(\boldsymbol{x}_n)\| &= \sqrt{\phi(\boldsymbol{x}^T)\phi(\boldsymbol{x}) + \phi(\boldsymbol{x}_n^T)\phi(\boldsymbol{x}_n) - 2\phi(\boldsymbol{x}^T)\phi(\boldsymbol{x}_n)} \\ &= \sqrt{k(\boldsymbol{x}, \boldsymbol{x}) + k(\boldsymbol{x}_n, \boldsymbol{x}_n) - 2k(\boldsymbol{x}, \boldsymbol{x}_n)} \end{aligned}$$

- So, the distance is now computed in a (hopefully) more convenient space.



- Note that we do not need to compute $\phi(\boldsymbol{x})$ and $\phi(\boldsymbol{x}_n)$.

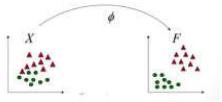
Support Vector Machines for Classification

- Consider binary classification with input space $\mathbb{R}^D$.
- Consider a training set $\{(\boldsymbol{x}_n, t_n)\}$ where $t_n \in \{-1, +1\}$.
- Consider using the linear model

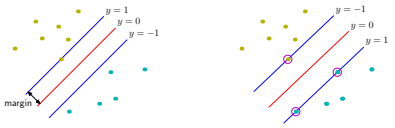
$$y(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x}) + b$$

so that a new point $\boldsymbol{x}$ is classified according to the sign of $y(\boldsymbol{x})$.

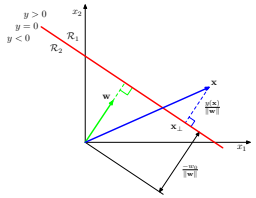
- Assume that the training set is linearly separable in the feature space (but not necessarily in the input space), i.e. $t_n y(\boldsymbol{x}_n) > 0$ for all n.



- Aim for the separating hyperplane that maximizes the margin (i.e. the smallest perpendicular distance from any point to the hyperplane) so as to minimize the generalization error.



Support Vector Machines for Classification



- The perpendicular distance from any point to the hyperplane is given by

$$\frac{t_n y(\boldsymbol{x}_n)}{\|\boldsymbol{w}\|} = \frac{t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b)}{\|\boldsymbol{w}\|}$$

- Then, the maximum margin separating hyperplane is given by

$$\arg\max_{\boldsymbol{w},b} \left(\min_n \frac{t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b)}{\|\boldsymbol{w}\|} \right)$$

- Multiply $\boldsymbol{w}$ and b by κ so that $t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b) = 1$ for the point closest to the hyperplane. Note that $t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b)/\|\boldsymbol{w}\|$ does not change.

Support Vector Machines for Classification

- Then, the maximum margin separating hyperplane is given by

$$\arg\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|^2$$

subject to $t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b) \geq 1$ for all n.

- To minimize the previous expression, we minimize

$$\frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_n a_n \big(t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b) - 1\big)$$

where $a_n \geq 0$ are called Lagrange multipliers.

- Note that any stationary point of the Lagrangian function is a stationary point of the original function subject to the constraints. Moreover, the Lagrangian function is a quadratic function subject to linear inequality constraints. Then, it is concave, actually concave up because of the +1/2 and, thus, "easy" to minimize.
- Note that we are now minimizing with respect to $\boldsymbol{w}$ and b, and maximizing with respect to a_n.
- Setting its derivatives with respect to $\boldsymbol{w}$ and b to zero gives

$$\boldsymbol{w} = \sum_n a_n t_n \phi(\boldsymbol{x}_n)$$

$$0 = \sum_n a_n t_n$$

Support Vector Machines for Classification

- Replacing the previous expressions in the Lagrangian function gives the dual representation of the problem, in which we maximize

$$\sum_n a_n - \frac{1}{2}\sum_n \sum_m a_n a_m t_n t_m \phi(\boldsymbol{x}_n)^T \phi(\boldsymbol{x}_m) = \sum_n a_n - \frac{1}{2}\sum_n \sum_m a_n a_m t_n t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

subject to $a_n \geq 0$ for all n, and $\sum_n a_n t_n = 0$.

- Again, this "easy" to maximize.
- Note that the dual representation makes use of the kernel trick, i.e. it allows working in a more convenient feature space without constructing it.

Support Vector Machines for Classification

- When the Lagrangian function is maximized, the Karush-Kuhn-Tucker condition holds for all n:

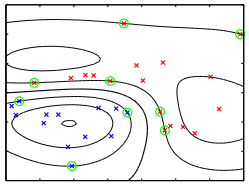
$$a_n(t_n y(\boldsymbol{x}_n) - 1) = 0$$

- Then, $a_n > 0$ if and only if $t_n y(\boldsymbol{x}_n) = 1$. The points with $a_n > 0$ are called support vectors and they lie on the margin boundaries.
- A new point $\boldsymbol{x}$ is classified according to the sign of

$$y(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x}) + b = \sum_n a_n t_n \phi(\boldsymbol{x}_n)^T \phi(\boldsymbol{x}) + b = \sum_n a_n t_n k(\boldsymbol{x}, \boldsymbol{x}_n) + b$$

$$= \sum_{m \in \mathcal{S}} a_m t_m k(\boldsymbol{x}, \boldsymbol{x}_m) + b$$

where $\mathcal{S}$ are the indexes of the support vectors. Sparse solution!



Support Vector Machines for Classification

- To find b, consider any support vector $\boldsymbol{x}_n$. Then,

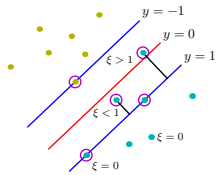
$$1 = t_n y(\boldsymbol{x}_n) = t_n\Big(\sum_{m \in \mathcal{S}} a_m t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m) + b\Big)$$

and multiplying both sides by t_n, we have that

$$b = t_n - \sum_{m \in \mathcal{S}} a_m t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

- We now drop the assumption of linear separability in the feature space, e.g. to avoid overfitting. We do so by introducing the slack variables $\xi_n \geq 0$ to penalize (almost-)misclassified points as

$$\xi_n = \begin{cases} 0 & \text{if } t_n y(\boldsymbol{x}_n) \geq 1 \\ |t_n - y(\boldsymbol{x}_n)| & \text{otherwise} \end{cases}$$

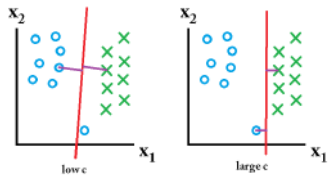


Support Vector Machines for Classification

- The optimal separating hyperplane is given by

$$\arg\min_{\boldsymbol{w},b,\{\xi_n\}} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_n \xi_n$$

subject to $t_n y(\boldsymbol{x}_n) \geq 1 - \xi_n$ and $\xi_n \geq 0$ for all n, and where $C > 0$ controls regularization. Its value can be decided by cross-validation. Note that the number of misclassified points is upper bounded by $\sum_n \xi_n$.



- To minimize the previous expression, we minimize

$$\frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_n \xi_n - \sum_n a_n\big(t_n(\boldsymbol{w}^T \phi(\boldsymbol{x}_n) + b) - 1 + \xi_n\big) - \sum_n \mu_n \xi_n$$

where $a_n \geq 0$ and $\mu_n \geq 0$ are Lagrange multipliers.

Support Vector Machines for Classification

- Setting its derivatives with respect to $\boldsymbol{w}$, b and ξ_n to zero gives

$$\boldsymbol{w} = \sum_n a_n t_n \phi(\boldsymbol{x}_n)$$

$$0 = \sum_n a_n t_n$$

$$a_n = C - \mu_n$$

- Replacing these in the Lagrangian function gives the dual representation of the problem, in which we maximize

$$\sum_n a_n - \frac{1}{2}\sum_n \sum_m a_n a_m t_n t_m k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

subject to $a_n \geq 0$ and $a_n \leq C$ for all n, because $\mu_n \geq 0$.

- When the Lagrangian function is maximized, the Karush-Kuhn-Tucker conditions hold for all n:

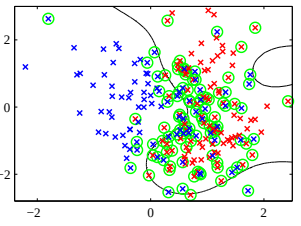
$$a_n(t_n y(\boldsymbol{x}_n) - 1 + \xi_n) = 0$$

$$\mu_n \xi_n = 0$$

- Then, $a_n > 0$ if and only if $t_n y(\boldsymbol{x}_n) = 1 - \xi_n$ for all n. The points with $a_n > 0$ are called support vectors and they lie
  - on the margin if $a_n < C$, because then $\mu_n > 0$ and thus $\xi_n = 0$, or
  - inside the margin (even on the wrong side of the decision boundary) if $a_n = C$, because then $\mu_n = 0$ and thus ξ_n is unconstrained.

Support Vector Machines for Classification

- Since the optimal $\boldsymbol{w}$ takes the same form as in the linearly separable case, classifying a new point is done the same as before. Finding b is done the same as before by considering any support vector $\boldsymbol{x}_n$ with $0 < a_n < C$.



- Not covered topics:
  - Classifying into more than two classes.
  - Returning class posterior probabilities.

Support Vector Machines for Regression

- Consider regressing an unidimensional continuous random variable on a D-dimensional continuous random variable.
- Consider a training set $\{(\boldsymbol{x}_n, t_n)\}$. Consider using the linear model

$$y(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x}) + b$$

- To get a sparse solution, instead of minimizing the classical regularized error function

$$\frac{1}{2}\sum_n (y(\boldsymbol{x}_n) - t_n)^2 + \frac{\lambda}{2}\|\boldsymbol{w}\|^2$$

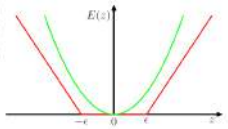
consider minimizing the ϵ-insensitive regularized error function

$$C\sum_n E_\epsilon(y(\boldsymbol{x}_n) - t_n) + \frac{1}{2}\|\boldsymbol{w}\|^2$$

where $C > 0$ controls regularization and

$$E_\epsilon(y(\boldsymbol{x}) - t) = \begin{cases} 0 & \text{if } |y(\boldsymbol{x}) - t| < \epsilon \\ |y(\boldsymbol{x}) - t| - \epsilon & \text{otherwise} \end{cases}$$

Figure 7.6 Plot of an ϵ-insensitive error function (in red) in which the error increases linearly with distance beyond the insensitive region. Also shown for comparison is the quadratic error function (in green).



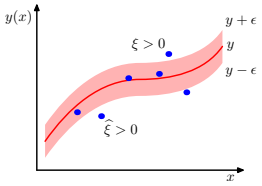
Support Vector Machines for Regression

- The values of C and ϵ can be decided by cross-validation.
- Consider the slack variables $\xi_n \geq 0$ and $\widehat{\xi}_n \geq 0$ such that

$$\xi_n = \begin{cases} t_n - y(\boldsymbol{x}_n) - \epsilon & \text{if } t_n > y(\boldsymbol{x}_n) + \epsilon \\ 0 & \text{otherwise} \end{cases}$$

and

$$\widehat{\xi}_n = \begin{cases} y(\boldsymbol{x}_n) - \epsilon - t_n & \text{if } t_n < y(\boldsymbol{x}_n) - \epsilon \\ 0 & \text{otherwise} \end{cases}$$



Support Vector Machines for Regression

- The optimal regression curve is given by

$$\arg\min_{\boldsymbol{w}, b, \{\xi_n\}, \{\widehat{\xi}_n\}} C\sum_n (\xi_n + \widehat{\xi}_n) + \frac{1}{2}\|\boldsymbol{w}\|^2$$

subject to $\xi \geq 0$, $\widehat{\xi}_n \geq 0$, $t_n \leq y(\boldsymbol{x}_n) + \epsilon + \xi_n$ and $t_n \geq y(\boldsymbol{x}_n) - \epsilon - \widehat{\xi}_n$.

- To minimize the previous expression, we minimize

$$C\sum_n (\xi_n + \widehat{\xi}_n) + \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_n (\mu_n \xi_n + \widehat{\mu}_n \widehat{\xi}_n)$$

$$- \sum_n a_n (y(\boldsymbol{x}_n) + \epsilon + \xi_n - t_n) - \sum_n \widehat{a}_n (t_n - y(\boldsymbol{x}_n) + \epsilon + \widehat{\xi}_n)$$

where $\mu_n \geq 0$, $\widehat{\mu}_n \geq 0$, $a_n \geq 0$ and $\widehat{a}_n \geq 0$ are Lagrange multipliers.

- Setting its derivatives with respect to $\boldsymbol{w}$, b, ξ_n and $\widehat{\xi}_n$ to zero gives

$$\boldsymbol{w} = \sum_n (a_n - \widehat{a}_n)\phi(\boldsymbol{x}_n)$$
$$0 = \sum_n (a_n - \widehat{a}_n)$$
$$C = a_n + \mu_n$$
$$C = \widehat{a}_n + \widehat{\mu}_n$$

Support Vector Machines for Regression

- Replacing these in the Lagrangian function gives the dual representation of the problem, in which we maximize

$$\frac{1}{2}\sum_n \sum_m (a_n - \widehat{a}_n)(a_m - \widehat{a}_m) k(\boldsymbol{x}_n, \boldsymbol{x}_m) - \epsilon \sum_n (a_n + \widehat{a}_n) + \sum_n (a_n - \widehat{a}_n) t_n$$

subject to $a_n \geq 0$ and $a_n \leq C$ for all n, because $\mu_n \geq 0$. Similarly for $\widehat{a}_n$.

- When the Lagrangian function is maximized, the Karush-Kuhn-Tucker conditions hold for all n:

$$a_n(y(\boldsymbol{x}_n) + \epsilon + \xi_n - t_n) = 0$$
$$\widehat{a}_n(t_n - y(\boldsymbol{x}_n) + \epsilon + \widehat{\xi}_n) = 0$$
$$\mu_n \xi_n = 0$$
$$\widehat{\mu}_n \widehat{\xi}_n = 0$$

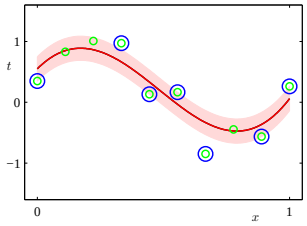
- Then, $a_n > 0$ if and only if $y(\boldsymbol{x}_n) + \epsilon + \xi_n - t_n = 0$, which implies that $\boldsymbol{x}_n$ lies on or above the upper margin of the ϵ-tube. Similarly for $\widehat{a}_n > 0$.

Support Vector Machines for Regression

- The prediction for a new point $\boldsymbol{x}$ is made according to

$$y(\boldsymbol{x}) = \sum_{m \in \mathcal{S}} (a_m - \widehat{a}_m) k(\boldsymbol{x}, \boldsymbol{x}_m) + b$$

where $\mathcal{S}$ are the indexes of the support vectors. Sparse solution!



- To find b, consider any support vector $\boldsymbol{x}_n$ with $0 < a_n < C$. Then, $\mu_n > 0$ and thus $\xi_n = 0$ and thus $0 = t_n - \epsilon - y(\boldsymbol{x}_n)$. Then,

$$b = t_n - \epsilon - \sum_{m \in \mathcal{S}} (a_m - \widehat{a}_m) k(\boldsymbol{x}_n, \boldsymbol{x}_m)$$

Neural Networks

- Consider binary classification with input space $\mathbb{R}^D$. Consider a training set $\{(\boldsymbol{x}_n, t_n)\}$ where $t_n \in \{-1, +1\}$.
- SVMs classify a new point $\boldsymbol{x}$ according to

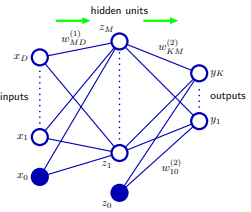
$$y(\boldsymbol{x}) = \text{sgn}\Big(\sum_{m\in\mathcal{S}} a_m t_m k(\boldsymbol{x}, \boldsymbol{x}_m) + b\Big)$$

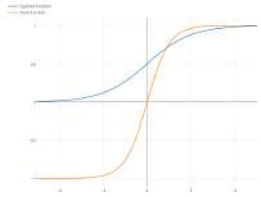
- Consider regressing an unidimensional continuous random variable on a D-dimensional continuous random variable. Consider a training set $\{(\boldsymbol{x}_n, t_n)\}$
- For a new point $\boldsymbol{x}$, SVMs predict

$$y(\boldsymbol{x}) = \sum_{m\in\mathcal{S}} (a_n - \widehat{a}_n) k(\boldsymbol{x}, \boldsymbol{x}_m) + b$$

- SVMs imply data-selected user-defined basis functions.
- NNs imply a user-defined number of data-selected basis functions.

Neural Networks





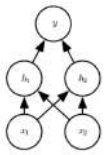
- Activations: $a_j = \sum_i w_{ji}^{(1)} x_i + w_{j0}^{(1)}$
- Hidden units and activation function: $z_j = h(a_j)$
- Output activations: $a_k = \sum_j w_{kj}^{(2)} z_j + w_{k0}^{(2)}$
- Output activation function for regression: $y_k(\boldsymbol{x}) = a_k$
- Output activation function for classification: $y_k(\boldsymbol{x}) = \sigma(a_k)$
- Sigmoid function: $\sigma(a) = \frac{1}{1+\exp(-a)}$
- Two-layer NN:

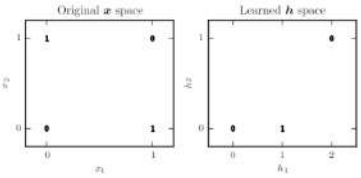
$$y_k(\boldsymbol{x}) = \sigma\Big(\sum_j w_{kj}^{(2)} h\Big(\sum_i w_{ji}^{(1)} x_i + w_{j0}^{(1)}\Big) + w_{k0}^{(2)}\Big)$$

- Evaluating the previous expression is known as forward propagation. The NN is said to have a feed-forward architecture.
- All the previous is, of course, generalizable to more layers.

Neural Networks

- Solving the XOR problem with NNs.
- No line shatters the points in the original space.
- The NN represents a mapping of the input space to an alternative space where a line can shatter the points. Note that the points (0,1) and (1,0) are mapped both to the point (1,0).
- **It resembles SVMs**.





$w_{11}^{(1)} = w_{12}^{(1)} = w_{21}^{(1)} = w_{22}^{(1)} = 1$
$w_{10}^{(1)} = 0,\ w_{20}^{(1)} = -1$
$h_j = z_j = h(a_j) = \max\{0, a_j\}$
$w_{11}^{(2)} = 1,\ w_{12}^{(2)} = -2$
$w_{10}^{(2)} = 0$
$y = y_k = a_k$

Backpropagation Algorithm

- Consider regressing an K-dimensional continuous random variable on a D-dimensional continuous random variable.
- Consider a training set $\{(\boldsymbol{x}_n, \boldsymbol{t}_n)\}$. Consider minimizing the sum-of-squares error function

$$E(\boldsymbol{w}) = \sum_n E_n(\boldsymbol{w}) = \sum_n \frac{1}{2}\|\boldsymbol{y}(\boldsymbol{x}_n) - \boldsymbol{t}_n\|^2 = \sum_n \sum_k \frac{1}{2}(y_k(\boldsymbol{x}_n) - t_{nk})^2$$

- This error function can be justified from a maximum likelihood approach to learning $\boldsymbol{w}$. To see it, **assume** that

$$p(t_k|\boldsymbol{x}, \boldsymbol{w}, \sigma) = \mathcal{N}(t_k|y_k(\boldsymbol{x}), \sigma)$$

- Then, the likelihood function is

$$p(\{\boldsymbol{t}_n\}|\{\boldsymbol{x}_n\}, \boldsymbol{w}, \sigma) = \prod_n \prod_k \mathcal{N}(t_{nk}|y_k(\boldsymbol{x}_n), \sigma) = \prod_n \prod_k \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{1}{2\sigma^2}(t_{nk} - y_k(\boldsymbol{x}_n))^2}$$

and thus

$$-\ln p(\{\boldsymbol{t}_n\}|\{\boldsymbol{x}_n\}, \boldsymbol{w}, \sigma) = \sum_n \sum_k \frac{1}{2\sigma^2}(t_{nk} - y_k(\boldsymbol{x}_n))^2 + \frac{N}{2}\ln\sigma^2 + \frac{N}{2}\ln 2\pi$$

which is equivalent to the sum-of-squares error function for a given σ.

- If σ is not given, then we can find the ML estimates of $\boldsymbol{w}$, plug them into the log likelihood function, and maximize it with respect to σ.

Backpropagation Algorithm

- The weight space is highly multimodal and, thus, we have to resort to approximate iterative methods to minimize the previous expression.
- Batch gradient descent

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \eta_t \nabla E(\boldsymbol{w}^t)$$

where $\eta_t > 0$ is the learning rate ($\sum_t \eta_t = \infty$ and $\sum_t \eta_t^2 < \infty$ to ensure convergence, e.g. $\eta_t = 1/t$).

- Sequential, stochastic or online gradient descent

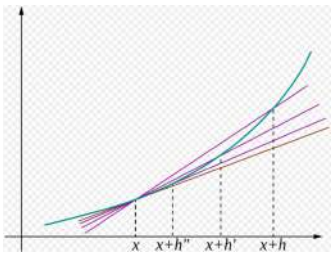
$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \eta_t \nabla E_n(\boldsymbol{w}^t)$$

where n is chosen randomly or sequentially.

- Sequential gradient descent is less affected by the multimodality problem, as a local minimum of the whole data will not be generally a local minimum of each individual point.

Backpropagation Algorithm

- Recall that $f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$

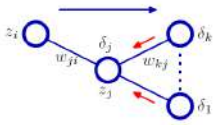


- Recall that $\nabla E_n(\boldsymbol{w}^t)$ is a vector whose components are the partial derivatives of $E_n(\boldsymbol{w}^t)$.

Backpropagation Algorithm

- Backpropagation algorithm:
  1. Forward propagate to compute activations, and hidden and output units.
  2. Compute δ_k for the output units.
  3. Backpropagate the δ's, i.e. evaluate δ_j for the hidden units recursively.
  4. Compute the required derivatives.

Figure 5.7 Illustration of the calculation of δ_j for hidden unit j by backpropagation of the δ's from those units k to which unit j sends connections. The blue arrow denotes the direction of information flow during forward propagation, and the red arrows indicate the backward propagation of error information.



- For classification, we minimize the negative log likelihood function, a.k.a. cross-entropy error function:

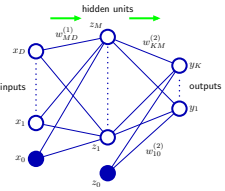
$$E_n(\boldsymbol{w}) = -\sum_k [t_{nk} \ln y_k(\boldsymbol{x}_n) + (1 - t_{nk}) \ln(1 - y_k(\boldsymbol{x}_n))]$$

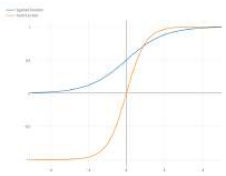
with $t_{nk} \in \{0, 1\}$ and $y_k(\boldsymbol{x}_n) = \sigma(a_k)$. Then, again

$$\frac{\partial E_n}{\partial w_{kj}} = \delta_k z_j \text{ and } \delta_k = \frac{\partial E_n}{\partial a_k} = y_k - t_k$$

- This is an example of embarrassingly parallel algorithm.

Backpropagation Algorithm





- Example: $y_k = a_k$, and $z_j = h(a_j) = \tanh(a_j)$ where $\tanh(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}$.
- Note that $h'(a) = 1 - h(a)^2$.
- Backpropagation:
  1. Forward propagation, i.e. compute
  $$a_j = \sum_i w_{ji} x_i \text{ and } z_j = h(a_j) \text{ and } y_k = \sum_j w_{kj} z_j$$
  2. Compute
  $$\delta_k = y_k - t_k$$
  3. Backpropagate, i.e. compute
  $$\delta_j = (1 - z_j^2) \sum_k w_{kj} \delta_k$$
  4. Compute
  $$\frac{\partial E_n}{\partial w_{kj}} = \delta_k z_j \text{ and } \frac{\partial E_n}{\partial w_{ji}} = \delta_j x_i$$

Backpropagation Algorithm

- The weight space is non-convex and has many symmetries, plateaus and local minima. So, the initialization of the weights in the backpropagation algorithm is crucial.
- Hints based on experimental rather than theoretical analysis:
  - Initialize the weights to different values, otherwise they would be updated in the same way because the algorithm is deterministic, and so creating redundant hidden units.
  - Initialize the weights at random, but
    - too small magnitude values may cause losing signal in the forward or backward passes, and
    - too big magnitude values may cause the activation function to saturate and lose gradient.
  - Initialize the weights according to prior knowledge: Almost-zero for hidden units that are unlikely to interact, and bigger magnitude values for the rest.
  - Initialize the weights to almost-zero values so that the initial model is almost-linear, i.e. the sigmoid function is almost-linear around the zero. Let the algorithm to introduce non-linearities where needed.
    - Note however that this initialization makes the sigmoid function take a value around half its saturation level. That is why the hyperbolic tangent function is sometimes preferred in practice.

Regularization

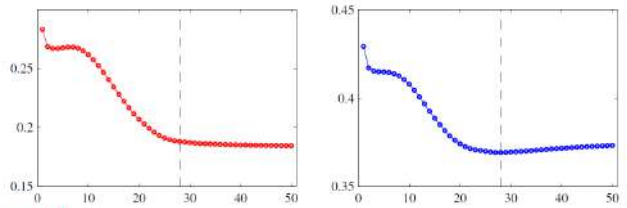


Figure 5.12 An illustration of the behaviour of training set error (left) and validation set error (right) during a typical training session, as a function of the iteration step, for the sinusoidal data set. The goal of achieving the best generalization performance suggests that training should be stopped at the point shown by the vertical dashed lines, corresponding to the minimum of the validation set error.

- Regularization when learning the parameters: Early stopping the backpropagation algorithm according to the error on some validation data.
- Regularization when learning the structure:
  - Cross-validation.
  - Penalizing complexity according to

$$E(\boldsymbol{w}) + \frac{\lambda}{2}\|\boldsymbol{w}\|^2 \text{ or } E(\boldsymbol{w}) + \frac{\lambda_1}{2}\|\boldsymbol{w}^{(1)}\|^2 + \frac{\lambda_2}{2}\|\boldsymbol{w}^{(2)}\|^2$$

and choose λ, or λ_1 and λ_2 by cross-validation. Note that the effect of the penalty is simply to add λw_{ji} and λw_{kj}, or $\lambda_1 w_{ji}$ and $\lambda_2 w_{kj}$ to the appropriate derivatives.

Limitations of Neural Networks

Theorem (Universal approximation theorem)

For every continuous function $f : [a, b]^D \to \mathbb{R}$ and for every $\epsilon > 0$, there exists a NN with one hidden layer such that

$$\sup_{\mathbf{x} \in [a,b]^D} |f(\mathbf{x}) - y(\mathbf{x})| < \epsilon$$

Theorem (Universal classification theorem)

Let $C^{(k)}$ contain all classifiers defined by NNs of one hidden layer with k hidden units and the sigmoid activation function. Then, for any distribution $p(\mathbf{x}, t)$,

$$\lim_{k \to \infty} \inf_{y \in C^{(k)}} L(y(\mathbf{x})) - L(p(t|\mathbf{x})) = 0$$

where $L()$ is the 0/1 loss function.

- How many hidden units has such a NN ?
- How much data do we need to learn such a NN (and avoid overfitting) via the backpropagation algorithm ?
- How fast does the backpropagation algorithm converge to such a NN ? Assuming that it does not get trapped in a local minimum...
- The answer to the last two questions depends on the first: More hidden units implies more training time and higher generalization error.

Limitations of Neural Networks

- How many hidden units does the NN need ?
- Any Boolean function can be written in disjunctive normal form (OR of ANDs) or conjunctive normal form (AND of ORs). This is a depth-two logical circuit.
- For most Boolean functions, the size of the circuit is exponential in the size of the input.
- However, there are Boolean functions that have a polynomial-size circuit of depth k and an exponential-size circuit of depth $k - 1$.
- Then, there is no universally right depth. Ideally, we should let the data determine the right depth.

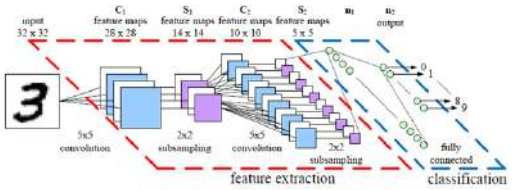
Theorem (No free lunch theorem)

For any algorithm, good performance on some problems comes at the expense of bad performance on some others.

Deep Neural Networks

- Training DNNs is difficult:
  - Typically, poorer generalization than (shallow) NNs.
  - The gradient may vanish/explode as we move away from the output layer, due to multiplying small/big quantities. E.g. the gradient of σ and tanh is in $[0, 1)$. So, they may only suffer the gradient vanishing problem. Other activations functions may suffer the gradient exploding problem.
  - There may be larger plateaus and many more local minima than with NNs.
- Training DNNs is doable:
  - Convolutional networks, particularly suitable for image processing.
  - Rectifier activation function, a new activation function.
  - Layer-wise pre-training, to find a good starting point for training.
- In addition to performance, the computational demands of the training must be considered, e.g. CPU, GPU, memory, parallelism, etc.
  - The authors state that GoogLeNet was trained "using modest amount of model and data-parallelism. Although we used a CPU based implementation only, a rough estimate suggests that the GoogLeNet network could be trained to convergence using few high-end GPUs within a week, the main limitation being the memory usage".

Convolutional Networks



- DNNs suitable for image recognition, since they exhibit invariance to translation, scaling, rotations, and warping.
- Convolution: Detection of local features, e.g. a_j is computed from a 5x5 pixel patch of the image.
- To achieve invariance, the units in the convolution layer share the same activation function and weights.
- Subsampling: Combination of local features into higher-order features, e.g. a_k is compute from a 2x2 pixel patch of the convoluted image.
- There are several feature maps in each layer, to compensate the reduction in resolution by increasing in the number of features being detected.
- The final layer is a regular NN for classification.

Convolutional Networks

- DNNs allow increased depth because
  - they are sparse, which allows the gradient to propagate further, and
  - they have relatively few weights to fit due to feature locality and weight sharing.
- The backpropagation algorithm needs to be adapted, by modifying the derivatives with respect to the weights in each convolution layer m.
- Since E_n depends on $w_i^{(m)}$ only via $a_j^{(m)}$, and $a_j^{(m)} = \sum_{i \in L_j^{(m)}} w_i^{(m)} z_i^{(m-1)}$ where $L_j^{(m)}$ is the set of indexes of the input units, then

$$\frac{\partial E_n}{\partial w_i^{(m)}} = \sum_j \frac{\partial E_n}{\partial a_j^{(m)}} \frac{\partial a_j^{(m)}}{\partial w_i^{(m)}} = \sum_j \delta_j^{(m)} z_i^{(m-1)}$$

- Note that $w_i^{(m)}$ does not depend on j by weight sharing, whereas $i \in L_j^{(m)}$ by feature locality.

Rectifier Activation Function

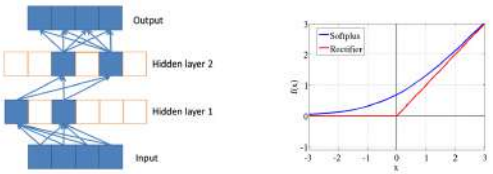


Figure 2: *Left:* **Sparse propagation of activations and gradients in a network of rectifier units.** The input selects a subset of active neurons and computation is linear in this subset. *Right:* **Rectifier and softplus activation functions.** The second one is a smooth version of the first.

- It simplifies the backpropagation algorithm as $h'(a_j) = 1$ for the selected units. So, there is no gradient vanishing on the paths of selected units. Compare with the sigmoid or hyperbolic tangent, for which
  - the gradient is smaller than one, or
  - even zero due to saturation.
- Note that $h'(0)$ does not exist since $h'_+(0) \neq h'_-(0)$. We can get around this problem by simply returning one of two one-sided derivatives. Or using a generalization of the rectifier function.
- Regularization is typically added to prevent numerical problems due to the activation being unbounded, e.g. when forward propagating.

Rectifier Activation Function

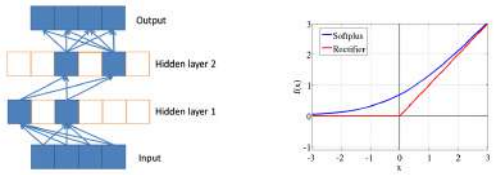


Figure 2: *Left:* **Sparse propagation of activations and gradients in a network of rectifier units.** The input selects a subset of active neurons and computation is linear in this subset. *Right:* **Rectifier and softplus activation functions.** The second one is a smooth version of the first.

- *rectifier*$(x) = \max\{0, x\}$, i.e. hidden units are off or operating in a linear regime.
- The most popular choice nowadays.
- Sparsity promoting: Uniform initialization of the weights implies that around 50 % of the hidden units are off.
- Piece-wise linear mapping: The input selects which hidden units are active, and the output is a liner function of the input in the selected hidden units.

Table of Common Distributions

taken from *Statistical Inference* by Casella and Berger

Discrete Distrbutions

distribution	pmf	mean	variance	mgf/moment
Bernoulli(p)	$p^x(1-p)^{1-x};\ x=0,1;\ p\in(0,1)$	p	$p(1-p)$	$(1-p)+pe^t$
Beta-binomial(n,α,β)	$\binom{n}{x}\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\frac{\Gamma(x+\alpha)\Gamma(n-x+\beta)}{\Gamma(\alpha+\beta+n)}$	$\frac{n\alpha}{\alpha+\beta}$	$\frac{n\alpha\beta}{(\alpha+\beta)^2}$	
Notes: If $X\|P$ is binomial (n,P) and P is beta(α,β), then X is beta-binomial(n,α,β).				
Binomial(n,p)	$\binom{n}{x}p^x(1-p)^{n-x};\ x=1,\ldots,n$	np	$np(1-p)$	$[(1-p)+pe^t]^n$
Discrete Uniform(N)	$\frac{1}{N};\ x=1,\ldots,N$	$\frac{N+1}{2}$	$\frac{(N+1)(N-1)}{12}$	$\frac{1}{N}\sum_{i=1}^{N}e^{it}$
Geometric(p)	$p(1-p)^{x-1};\ p\in(0,1)$	$\frac{1}{p}$	$\frac{1-p}{p^2}$	$\frac{pe^t}{1-(1-p)e^t}$
Note: $Y=X-1$ is negative binomial$(1,p)$. The distribution is *memoryless*: $P(X>s\|X>t)=P(X>s-t)$.				
Hypergeometric(N,M,K)	$\frac{\binom{M}{x}\binom{N-M}{K-x}}{\binom{N}{K}};\ x=1,\ldots,K$	$\frac{KM}{N}$	$\frac{KM}{N}\frac{(N-M)(N-k)}{N(N-1)}$	?
	$M-(N-K)\le x\le M;\ N,M,K>0$			
Negative Binomial(r,p)	$\binom{r+x-1}{x}p^r(1-p)^x;\ p\in(0,1)$	$\frac{r(1-p)}{p}$	$\frac{r(1-p)}{p^2}$	$\left(\frac{p}{1-(1-p)e^t}\right)^r$
	$\binom{y-1}{r-1}p^r(1-p)^{y-r};\ Y=X+r$			
Poisson(λ)	$\frac{e^{-\lambda}\lambda^x}{x!};\ \lambda\ge0$	λ	λ	$e^{\lambda(e^t-1)}$
Notes: If Y is gamma(α,β), X is Poisson$(\frac{x}{\beta})$, and α is an integer, then $P(X\ge\alpha)=P(Y\le y)$.				

Continuous Distributions

distribution	pdf	mean	variance	mgf/moment
Beta(α,β)	$\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}x^{\alpha-1}(1-x)^{\beta-1};\ x\in(0,1),\ \alpha,\beta>0$	$\frac{\alpha}{\alpha+\beta}$	$\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$	$1+\sum_{k=1}^{\infty}\left(\prod_{r=0}^{k-1}\frac{\alpha+r}{\alpha+\beta+r}\right)\frac{t^k}{k!}$
Cauchy(θ,σ)	$\frac{1}{\pi\sigma}\frac{1}{1+(\frac{x-\theta}{\sigma})^2};\ \sigma>0$	does not exist	does not exist	does not exist
Notes: Special case of Students's t with 1 degree of freedom. Also, if X,Y are iid $N(0,1)$, $\frac{X}{Y}$ is Cauchy				
χ^2_p	$\frac{1}{\Gamma(\frac{p}{2})2^{\frac{p}{2}}}x^{\frac{p}{2}-1}e^{-\frac{x}{2}};\ x>0,\ p\in N$	p	$2p$	$\left(\frac{1}{1-2t}\right)^{\frac{p}{2}},\ t<\frac{1}{2}$
Notes: Gamma$(\frac{p}{2},2)$.				
Double Exponential(μ,σ)	$\frac{1}{2\sigma}e^{-\frac{\lvert x-\mu\rvert}{\sigma}};\ \sigma>0$	μ	$2\sigma^2$	$\frac{e^{\mu t}}{1-(\sigma t)^2}$
Exponential(θ)	$\frac{1}{\theta}e^{-\frac{x}{\theta}};\ x\geq 0,\ \theta>0$	θ	θ^2	$\frac{1}{1-\theta t},\ t<\frac{1}{\theta}$
Notes: Gamma$(1,\theta)$. Memoryless. $Y=X^{\frac{1}{\gamma}}$ is *Weibull*. $Y=\sqrt{\frac{2X}{\beta}}$ is *Rayleigh*. $Y=\alpha-\gamma\log\frac{X}{\beta}$ is *Gumbel*.				
F_{ν_1,ν_2}	$\frac{\Gamma(\frac{\nu_1+\nu_2}{2})}{\Gamma(\frac{\nu_1}{2})\Gamma(\frac{\nu_2}{2})}\left(\frac{\nu_1}{\nu_2}\right)^{\frac{\nu_1}{2}}\frac{x^{\frac{\nu_1-2}{2}}}{\left(1+(\frac{\nu_1}{\nu_2})x\right)^{\frac{\nu_1+\nu_2}{2}}};\ x>0$	$\frac{\nu_2}{\nu_2-2},\ \nu_2>2$	$2(\frac{\nu_2}{\nu_2-2})^2\frac{\nu_1+\nu_2-2}{\nu_1(\nu_2-4)},\ \nu_2>4$	$EX^n=\frac{\Gamma(\frac{\nu_1+2n}{2})\Gamma(\frac{\nu_2-2n}{2})}{\Gamma(\frac{\nu_1}{2})\Gamma(\frac{\nu_2}{2})}\left(\frac{\nu_2}{\nu_1}\right)^n,\ n<\frac{\nu_2}{2}$
Notes: $F_{\nu_1,\nu_2}=\frac{\chi^2_{\nu_1}/\nu_1}{\chi^2_{\nu_2}/\nu_2}$, where the χ^2s are independent. $F_{1,\nu}=t^2_\nu$.				
Gamma(α,β)	$\frac{1}{\Gamma(\alpha)\beta^\alpha}x^{\alpha-1}e^{-\frac{x}{\beta}};\ x>0,\ \alpha,\beta>0$	$\alpha\beta$	$\alpha\beta^2$	$\left(\frac{1}{1-\beta t}\right)^\alpha,\ t<\frac{1}{\beta}$
Notes: Some special cases are exponential ($\alpha=1$) and χ^2 ($\alpha=\frac{p}{2},\beta=2$). If $\alpha=\frac{2}{3},\ Y=\sqrt{\frac{X}{\beta}}$ is *Maxwell*. $Y=\frac{1}{X}$ is *inverted gamma*.				
Logistic(μ,β)	$\frac{1}{\beta}\frac{e^{-\frac{x-\mu}{\beta}}}{\left[1+e^{-\frac{x-\mu}{\beta}}\right]^2};\ \beta>0$	μ	$\frac{\pi^2\beta^2}{3}$	$e^{\mu t}\Gamma(1+\beta t),\ \lvert t\rvert<\frac{1}{\beta}$
Notes: The cdf is $F(x\lvert\mu,\beta)=\frac{1}{1+e^{-\frac{x-\mu}{\beta}}}$.				
Lognormal(μ,σ^2)	$\frac{1}{\sqrt{2\pi}\sigma}\frac{1}{x}e^{-\frac{(\log x-\mu)^2}{2\sigma^2}};\ x>0,\sigma>0$	$e^{\mu+\frac{\sigma^2}{2}}$	$e^{2(\mu+\sigma^2)}-e^{2\mu+\sigma^2}$	$EX^n=e^{n\mu+\frac{n^2\sigma^2}{2}}$
Normal(μ,σ^2)	$\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu)^2}{2\sigma^2}};\ \sigma>0$	μ	σ^2	$e^{\mu t+\frac{\sigma^2t^2}{2}}$
Pareto(α,β)	$\frac{\beta\alpha^\beta}{x^{\beta+1}};\ x>\alpha,\ \alpha,\beta>0$	$\frac{\beta\alpha}{\beta-1},\ \beta>1$	$\frac{\beta\alpha^2}{(\beta-1)^2(\beta-2)},\ \beta>2$	does not exist
t_ν	$\frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})}\frac{1}{\sqrt{\nu\pi}}\frac{1}{(1+\frac{x^2}{\nu})^{\frac{\nu+1}{2}}}$	$0,\ \nu>1$	$\frac{\nu}{\nu-2},\nu>2$	$EX^n=\frac{\Gamma(\frac{\nu+1}{2})\Gamma(\nu-\frac{n}{2})}{\sqrt{\pi}\Gamma(\frac{\nu}{2})}\nu^{\frac{n}{2}},\ n$ even
Notes: $t^2_\nu=F_{1,\nu}$.				
Uniform(a,b)	$\frac{1}{b-a},\ a\leq x\leq b$	$\frac{b+a}{2}$	$\frac{(b-a)^2}{12}$	$\frac{e^{bt}-e^{at}}{(b-a)t}$
Notes: If $a=0,\ b=1$, this is special case of beta ($\alpha=\beta=1$).				
Weibull(γ,β)	$\frac{\gamma}{\beta}x^{\gamma-1}e^{-\frac{x^\gamma}{\beta}};\ x>0,\ \gamma,\beta>0$	$\beta^{\frac{1}{\gamma}}\Gamma(1+\frac{1}{\gamma})$	$\beta^{\frac{2}{\gamma}}\left[\Gamma(1+\frac{2}{\gamma})-\Gamma^2(1+\frac{1}{\gamma})\right]$	$EX^n=\beta^{\frac{n}{\gamma}}\Gamma(1+\frac{n}{\gamma})$
Notes: The mgf only exists for $\gamma\geq 1$.				