Lab 4 complementary assignment

Anton Persson antpe404

21 januari 2017

Complimentary assignment for lab 4 732A95

The task I was about to do as a complimentary assignment was formulated as *Use NIRspectra.xls and Viscosity as a target variable in order to implement a linear regression model in which features are first M components in ICA analysis. Provide a plot showing a mean square prediction error of this model (cross-validation error) versus number of ICA features selected. Compare with a corresponding ´plot in lab 4 and make conclusions.*

I start off by answering the first question, by implementing a linear regression model in which features are first M component in ICA analysis. The code is shown below. Note that I'm using the fastICA() function from the package with the same name to do the ICA analysis.

```
library(ggplot2)
library(fastICA)
```

```
## Warning: package 'fastICA' was built under R version 3.3.2
```

```
nir<-read.csv2("data/NIRspectra.csv", sep=";", header=T)

part_one<-function(data=nir, y=Viscosity, M=3){
  #data=nir
  #y="Viscosity"
  #M=3

  new_x<-data.frame(fastICA(data, n.comp=M)$S) #Extraherar M ICA components.
  newdata<-cbind(Viscosity=data$Viscosity, new_x)
  formula<-as.formula(paste("Viscosity~", paste(colnames(newdata)[-1], collapse="+")))

  des.mat<-model.matrix(formula, newdata)
  dep.var <- all.vars(formula)[1]
  dep.var <- as.matrix(nir[dep.var])
  beta.hat <- solve( t(des.mat) %*% des.mat )  %*% t(des.mat) %*% dep.var
  y.hat <- des.mat %*% beta.hat
  res.err <- dep.var - y.hat
  degree.free <- nrow(des.mat) - ncol(des.mat)
  res.var2 <-( t(res.err) %*% res.err ) / degree.free
  var.hat.bhat <-diag( as.vector(res.var2) *  solve( t(des.mat) %*% des.mat )  )
  t.beta <- beta.hat / sqrt( var.hat.bhat )
  my.pvalues<- (1 - pt( abs( t.beta ) ,df = degree.free) ) * 2

  l<-list(coefficients = t(beta.hat) , degree.free = degree.free, res.var2 = res.var2,
          var.hat.bhat = var.hat.bhat, t.beta = t.beta, my.pvalues = my.pvalues,
          formula = formula, dataset=deparse(substitute(data)),
           data=cbind(des.mat,dep.var),y.hat=y.hat,res.err=res.err)
  return(l$coefficients)
}

part_one()
```

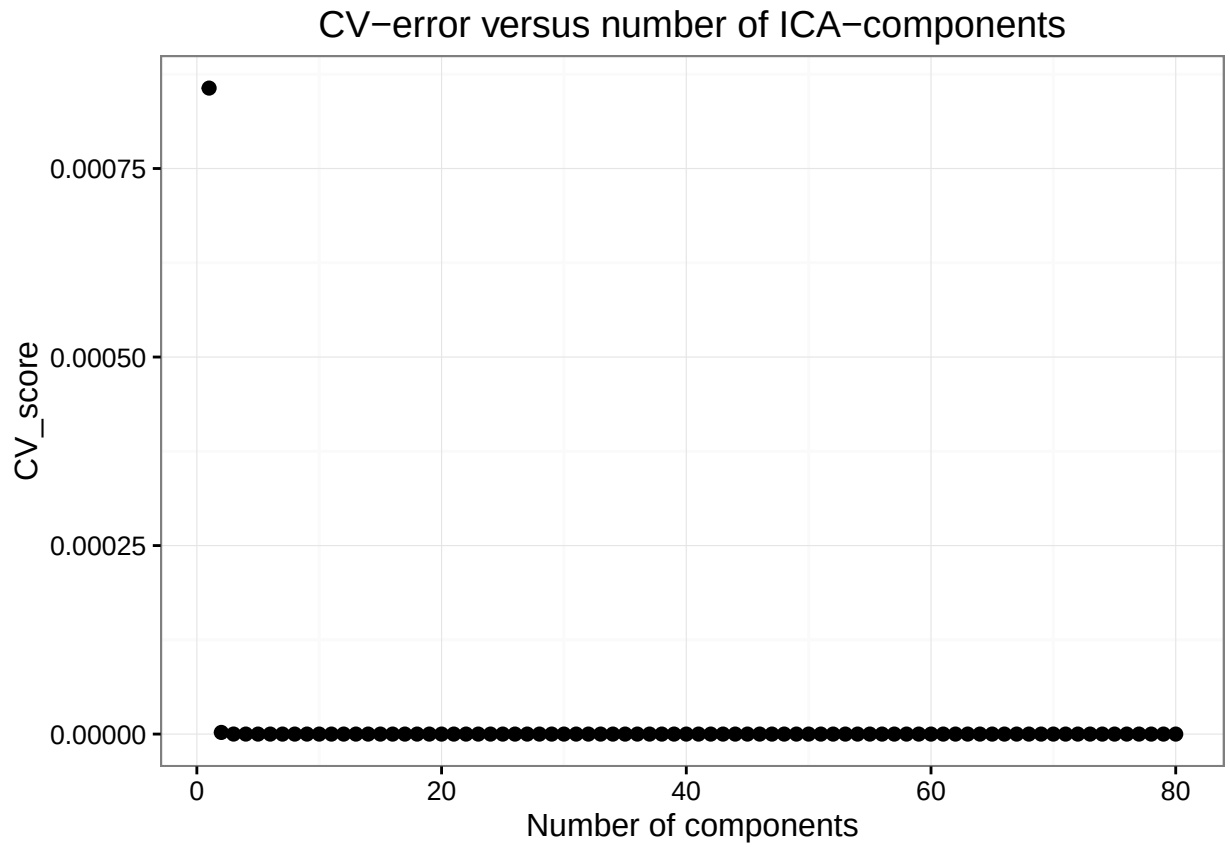
```
##           (Intercept)          X1          X2         X3
## Viscosity    2.516911 -0.05830962 -0.02467664 -0.5239376
```

In the code chunk above I chose to show only the coefficients for the model when the number of ICA components equals 3. As you can see, from this function I could show almost any values that might be of interest.

For the second part of the question, to run the function over several different values of M and plot their cross validation error versus the number of components, the following code is used.

```
CV_ica <- function(data=nir, folds, M) {
  Y<-data$Viscosity
  Y<-as.matrix(Y)
  CV<-integer(0)
  resmat<-matrix(ncol=M, nrow=folds)

  for (j in 1:M){

    X<-data.frame(fastICA(data, n.comp=(j))$S) #Extraherar M ICA components.
    X<-as.matrix(X)

    n<-dim(X)[1]
    X<-cbind(rep(1, n), X)#Intercept-ettorna for X-matrisen
    p<-dim(X)[2]

    for (i in 1:folds){
      slumpat<-as.vector(unlist(suppressWarnings(split(1:n, f=1:folds)[i])))

      test<-X[slumpat, 1:(j+1)] #+1 eftersom jag har interceptcol
      train<-X[-slumpat, 1:(j+1)]
      Y_test<-Y[slumpat, ]
      Y_train<-Y[-slumpat, ]

      betahat<-solve(t(train)%*%train) %*% t(train) %*% Y_train #Skattar modellen pa traningsdatan
      yhat <- test %*% betahat  #Testar pa den nya datan, dvs skattar nya datan.
      resid_err <- Y_test - yhat #Och tar fram felen.

      CV[i]<-sum(resid_err**2)
    }
    resmat[,j]<-CV
  }
  resmat<-as.data.frame(resmat)
  CV_score<-apply(resmat, 2, mean)
  data<-as.data.frame(cbind(CV_score, M=1:M))
  #data<-as.data.frame(cbind(log_cv=log(CV_score), M=1:M))

  cv_plotten<-ggplot(data=data)+geom_point(aes(x=M, y=CV_score), size=2)+#y=log_cv
    theme_bw()+
    #ylim(c(0,.001))+
    xlab("Number of components")+
    ggtitle("CV-error versus number of ICA-components")#+
    #geom_hline(yintercept=min(data$CV_score), col="red")

  optimal_subset<-data[data$CV_score==min(data$CV_score),]
```

```
  plot(cv_plotten)
  #return(data)
  return(optimal_subset)
}

CV_ica(data=nir, folds=3, M=80)
```




```
##         CV_score  M
## V80 3.102878e-15 80
```