AEs

```
library(keras)
library(RColorBrewer)
library(caret)
```

```
## Loading required package: lattice
```

```
## Loading required package: ggplot2
```

```
library(readr)
library(pROC)
```

```
## Type 'citation("pROC")' for a citation.
```

```
##
## Attaching package: 'pROC'
```

```
## The following objects are masked from 'package:stats':
##
##     cov, smooth, var
```

```
setwd("~/Docencia/curs21_22/UB/MESIO/DL/unitat3/Breast")
clinical <- read_delim("clinical.csv","\t", escape_double = FALSE, trim_ws = TRUE)
```

```
##
## -- Column specification --------------------------------------------------------
## cols(
##   Sample = col_character(),
##   Histology = col_character(),
##   PAM50Call = col_character(),
##   ajcc_cancer_metastasis_stage_code = col_character(),
##   ajcc_neoplasm_disease_lymph_node_stage = col_character(),
##   ajcc_neoplasm_disease_stage = col_character(),
##   ajcc_tumor_stage_code = col_character(),
##   breast_cancer_optical_measurement_histologic_type = col_character(),
##   breast_carcinoma_estrogen_receptor_status = col_character(),
##   breast_carcinoma_progesterone_receptor_status = col_character(),
##   breast_carcinoma_surgical_procedure_name = col_character(),
##   gender = col_character(),
##   her2_immunohistochemistry_level_result = col_character(),
##   lab_proc_her2_neu_immunohistochemistry_receptor_status = col_character(),
##   margin_status = col_character(),
##   menopause_status = col_character(),
##   person_neoplasm_cancer_status = col_character(),
##   sample_type = col_character(),
##   vital_status = col_character()
## )
```

```
#gene_expression <- read_delim("gene_expression.csv","\t", escape_double = FALSE, trim_ws = TRUE)
protein_abundance <- read_delim("protein_abundance.csv","\t", escape_double = FALSE, trim_ws = TRUE)
```

```
##
## -- Column specification --------------------------------------------------------
## cols(
##   .default = col_double(),
##   Sample = col_character()
## )
## i Use `spec()` for the full column specifications.
```

```
#copy_number <- read_delim("copy_number.csv","\t", escape_double = FALSE, trim_ws = TRUE)

set1<-intersect(protein_abundance$Sample,clinical$Sample)

xclinical<-clinical[clinical$Sample%in%set1,]
xprotein<-protein_abundance[protein_abundance$Sample%in%set1,]

xclinical<-xclinical[,c(1,9)]
sel1<-which(xclinical$breast_carcinoma_estrogen_receptor_status!="Positive")
sel2<-which(xclinical$breast_carcinoma_estrogen_receptor_status!="Negative")

sel<-intersect(sel1,sel2)
xclinical<-xclinical[-sel,]

xclinical<-xclinical[-which(is.na(xclinical$breast_carcinoma_estrogen_receptor_status)),]


mprotein<-merge(xclinical,xprotein,by.x="Sample",by.y="Sample")


# pprotein
sel<-complete.cases(t(mprotein))
```

```
set.seed(111)
training<-sample(1:nrow(mprotein),2*nrow(mprotein)/3)


xtrain<-mprotein[training,-c(1,2)]
xtest<-mprotein[-training,-c(1,2)]

xtrain<-scale(xtrain)
xtest<-scale(xtest)

ytrain<-mprotein[training,2]
ytest<-mprotein[-training,2]

ylabels<-vector()
ylabels[ytrain=="Positive"]<-1
ylabels[ytrain=="Negative"]<-0


ytestlabels<-vector()
ytestlabels[ytest=="Positive"]<-1
ytestlabels[ytest=="Negative"]<-0
```

Autoencoder

```
model<-keras_model_sequential() %>%
  layer_dense(units=50,activation="relu",input_shape=c(142)) %>%
  layer_dense(units=20,activation="relu") %>%
  layer_dense(units=50,activation="relu") %>%
  layer_dense(units=142,activation="linear")
```

```
summary(model)
```

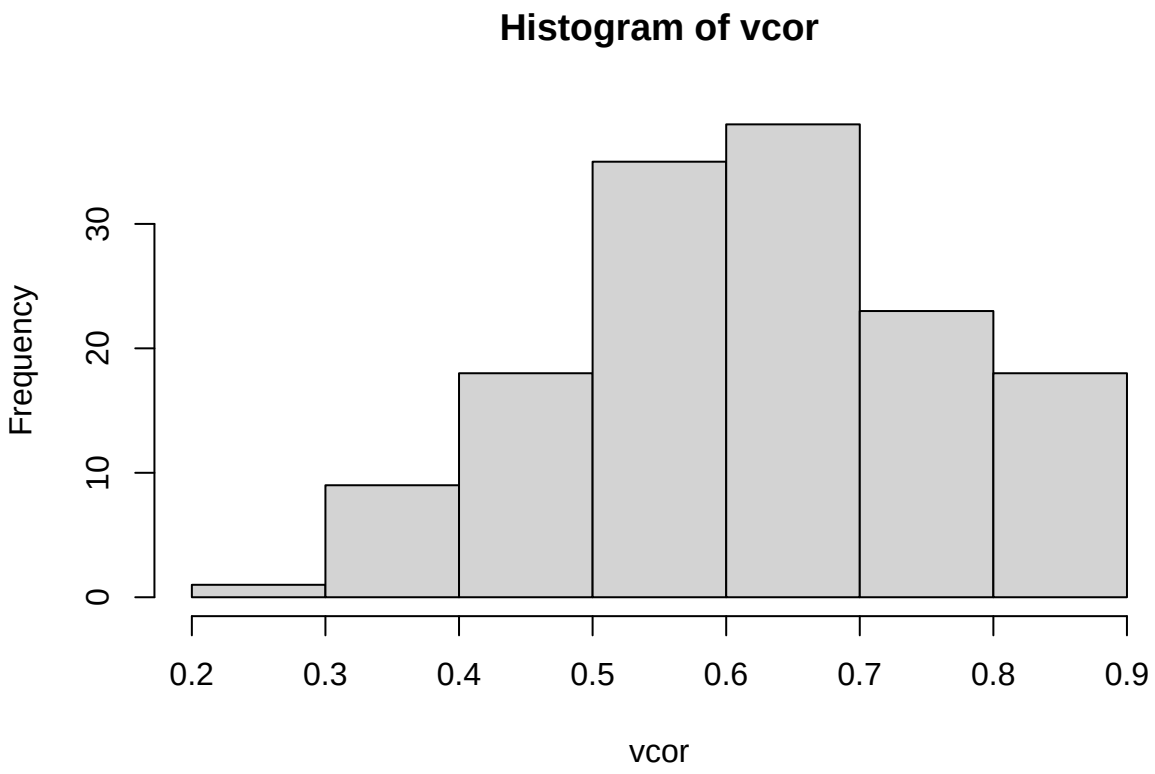
```
## Model: "sequential"
## _________________________________________________________________________________
## Layer (type)                        Output Shape                    Param #
## =================================================================================
## dense_3 (Dense)                     (None, 50)                      7150
## _________________________________________________________________________________
## dense_2 (Dense)                     (None, 20)                      1020
## _________________________________________________________________________________
## dense_1 (Dense)                     (None, 50)                      1050
## _________________________________________________________________________________
## dense (Dense)                       (None, 142)                     7242
## =================================================================================
## Total params: 16,462
## Trainable params: 16,462
## Non-trainable params: 0
## _________________________________________________________________________________
```

```
model %>% compile(
  optimizer = "rmsprop",
  loss = "mse"
)
```

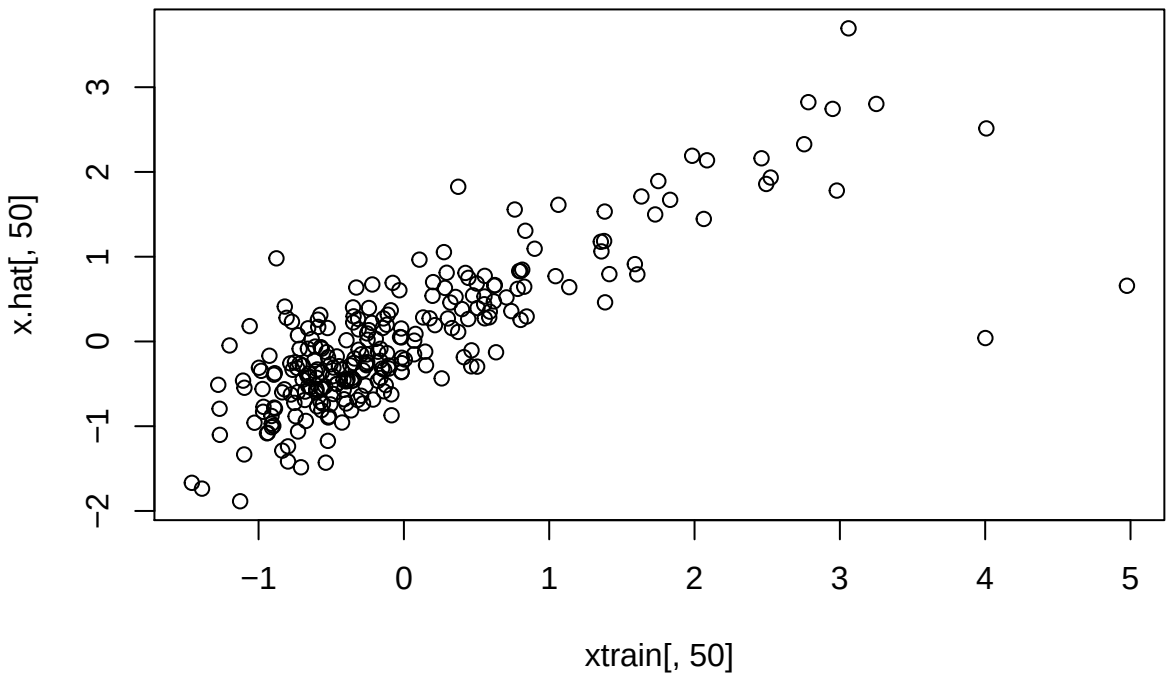
```
model %>% fit(
  x=as.matrix(xtrain),
  y=as.matrix(xtrain),
  epochs = 25,
  batch_size=64,
  validation_split = 0.2
  )
```

```
x.hat<-predict(model,as.matrix(xtrain))
```

```
vcor<-diag(cor(x.hat,xtrain))
hist(vcor)
```

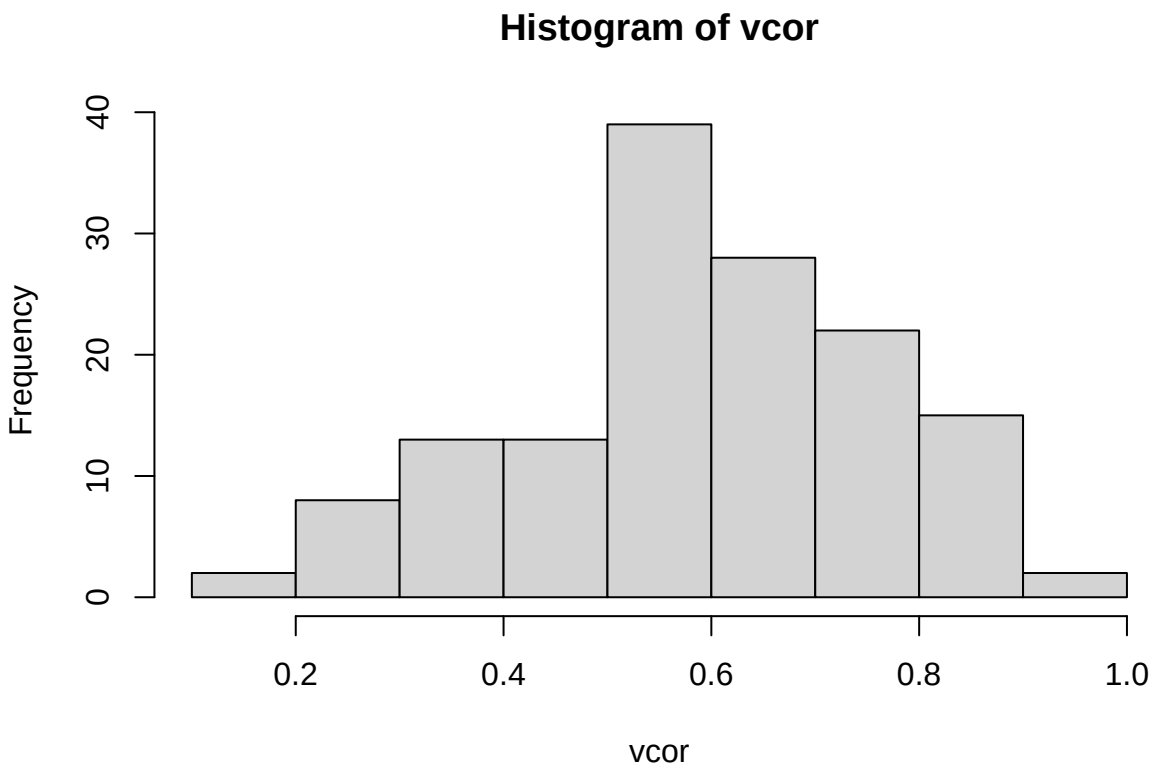



```
# visual inspection
plot(x.hat[,50]~xtrain[,50])
```

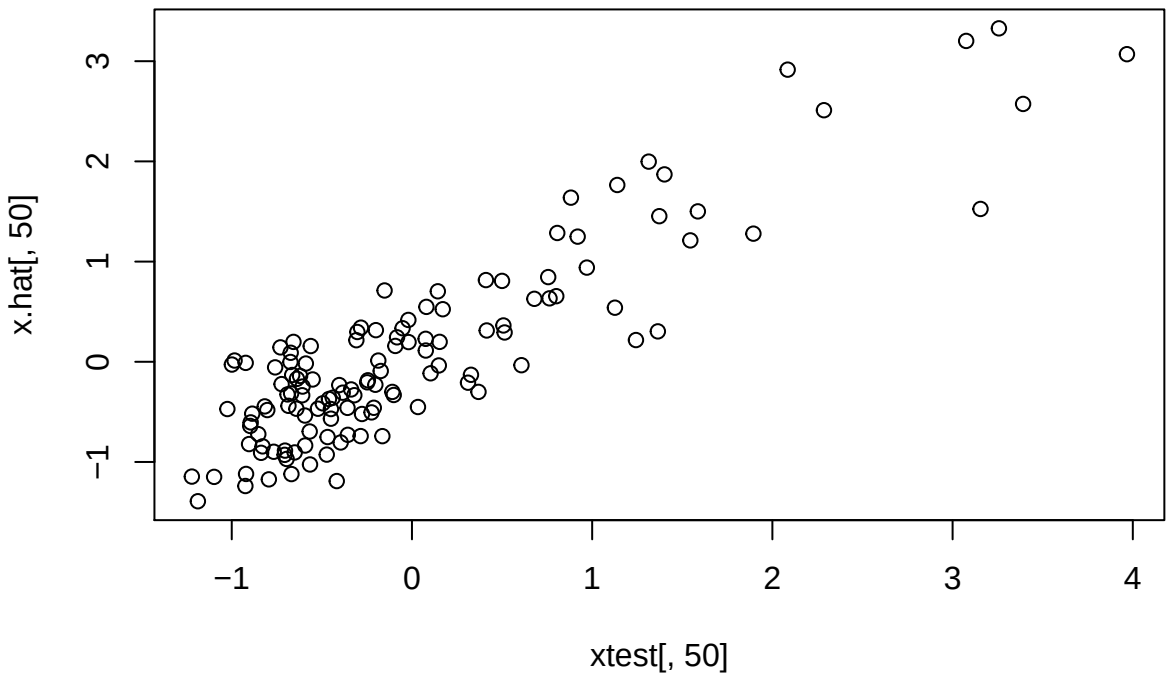



```
x.hat<-predict(model,as.matrix(xtest))
```

```
vcor<-diag(cor(x.hat,xtest))
hist(vcor)
```




```
# visual inspection
plot(x.hat[,50]~xtest[,50])
```



Defining Encoder and Decoder submodels

```
input_enc<-layer_input(shape = 142)
output_enc<-input_enc %>%
  layer_dense(units=50,activation="relu") %>%
  layer_dense(units=20,activation="relu")

encoder = keras_model(input_enc, output_enc)
summary(encoder)
```

```
## Model: "model"
## _________________________________________________________________________
## Layer (type)                 Output Shape              Param #
## =========================================================================
## input_1 (InputLayer)         [(None, 142)]             0
## _________________________________________________________________________
## dense_5 (Dense)              (None, 50)                7150
## _________________________________________________________________________
## dense_4 (Dense)              (None, 20)                1020
## =========================================================================
## Total params: 8,170
## Trainable params: 8,170
## Non-trainable params: 0
## _________________________________________________________________________
```

```
input_dec = layer_input(shape = 20)
output_dec<-input_dec %>%
  layer_dense(units=50,activation="relu") %>%
  layer_dense(units=142,activation="linear")

decoder = keras_model(input_dec, output_dec)

summary(decoder)
```

```
## Model: "model_1"
## _________________________________________________________________________
## Layer (type)                    Output Shape                  Param #
## =========================================================================
## input_2 (InputLayer)            [(None, 20)]                  0
## _________________________________________________________________________
## dense_7 (Dense)                 (None, 50)                    1050
## _________________________________________________________________________
## dense_6 (Dense)                 (None, 142)                   7242
## =========================================================================
## Total params: 8,292
## Trainable params: 8,292
## Non-trainable params: 0
## _________________________________________________________________________
```

Defining Autoencoder

```
aen_input = layer_input(shape = 142)
aen_output = aen_input %>%
  encoder() %>%
  decoder()

aen = keras_model(aen_input, aen_output)
summary(aen)
```

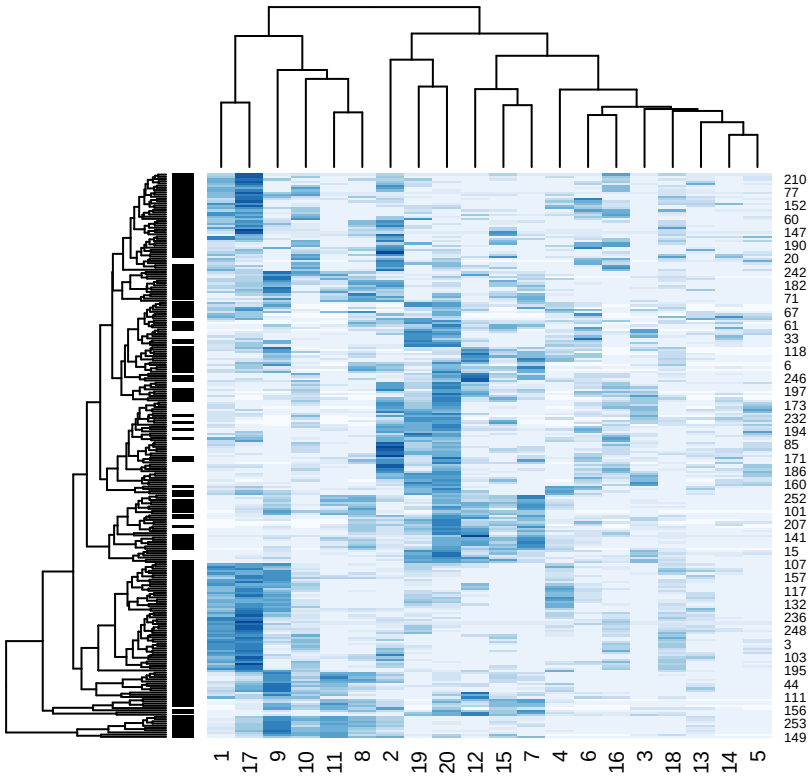
```
## Model: "model_2"
## _________________________________________________________________________
## Layer (type)                    Output Shape                  Param #
## =========================================================================
## input_3 (InputLayer)            [(None, 142)]                 0
## _________________________________________________________________________
## model (Model)                   (None, 20)                    8170
## _________________________________________________________________________
## model_1 (Model)                 (None, 142)                   8292
## =========================================================================
## Total params: 16,462
## Trainable params: 16,462
## Non-trainable params: 0
## _________________________________________________________________________
```

```
aen %>% compile(
  optimizer = "rmsprop",
  loss = "mse"
)
```

```
aen %>% fit(
  x=as.matrix(xtrain),
  y=as.matrix(xtrain),
  epochs = 25,
  batch_size=64,
  validation_split = 0.2
  )
```

```
#Generating with Autoencoder
encoded_expression <- encoder %>% predict(as.matrix(xtrain))
decoded_expression <- decoder %>% predict(encoded_expression)
```

```
colMain <- colorRampPalette(brewer.pal(8, "Blues"))(15)
heatmap(encoded_expression,  RowSideColors=as.character(ylabels) , col=colMain, scale="row" )
```



Stacked autoencoder

AE1

```
input_enc1<-layer_input(shape = 142)
output_enc1<-input_enc1 %>%
  layer_dense(units=50,activation="relu")
encoder1 = keras_model(input_enc1, output_enc1)
summary(encoder1)
```

```
## Model: "model_3"
## ________________________________________________________________________________
```

```
## Layer (type)                 Output Shape              Param #
## ================================================================================
## input_4 (InputLayer)         [(None, 142)]             0
## ________________________________________________________________________________
## dense_8 (Dense)              (None, 50)                7150
## ================================================================================
## Total params: 7,150
## Trainable params: 7,150
## Non-trainable params: 0
## ________________________________________________________________________________
```

```
input_dec1 = layer_input(shape = 50)
output_dec1<-input_dec1 %>%
  layer_dense(units=142,activation="linear")

decoder1 = keras_model(input_dec1, output_dec1)

summary(decoder1)
```

```
## Model: "model_4"
## ________________________________________________________________________________
## Layer (type)                 Output Shape              Param #
## ================================================================================
## input_5 (InputLayer)         [(None, 50)]              0
## ________________________________________________________________________________
## dense_9 (Dense)              (None, 142)               7242
## ================================================================================
## Total params: 7,242
## Trainable params: 7,242
## Non-trainable params: 0
## ________________________________________________________________________________
```

```
aen_input1 = layer_input(shape = 142)
aen_output1 = aen_input1 %>%
  encoder1() %>%
  decoder1()

sae1 = keras_model(aen_input1, aen_output1)
summary(sae1)
```

```
## Model: "model_5"
## ________________________________________________________________________________
## Layer (type)                 Output Shape              Param #
## ================================================================================
## input_6 (InputLayer)         [(None, 142)]             0
## ________________________________________________________________________________
## model_3 (Model)              (None, 50)                7150
## ________________________________________________________________________________
## model_4 (Model)              (None, 142)               7242
## ================================================================================
## Total params: 14,392
## Trainable params: 14,392
## Non-trainable params: 0
## ________________________________________________________________________________
```

```
sae1 %>% compile(
  optimizer = "rmsprop",
  loss = "mse"
)
```

```
sae1 %>% fit(
  x=as.matrix(xtrain),
  y=as.matrix(xtrain),
  epochs = 25,
  batch_size=64,
  validation_split = 0.2
  )
```

```
#Generating with Autoencoder
encoded_expression1 <- encoder1 %>% predict(as.matrix(xtrain))
```

AE2

```
input_enc2<-layer_input(shape = 50)
output_enc2<-input_enc2 %>%
  layer_dense(units=20,activation="relu")
encoder2 = keras_model(input_enc2, output_enc2)
summary(encoder2)
```

```
## Model: "model_6"
## _________________________________________________________________________________
## Layer (type)                    Output Shape                  Param #
## =================================================================================
## input_7 (InputLayer)            [(None, 50)]                  0
## _________________________________________________________________________________
## dense_10 (Dense)                (None, 20)                    1020
## =================================================================================
## Total params: 1,020
## Trainable params: 1,020
## Non-trainable params: 0
## _________________________________________________________________________________
```

```
input_dec2 = layer_input(shape = 20)
output_dec2<-input_dec2 %>%
  layer_dense(units=50,activation="linear")

decoder2 = keras_model(input_dec2, output_dec2)

summary(decoder2)
```

```
## Model: "model_7"
## _________________________________________________________________________________
## Layer (type)                    Output Shape                  Param #
## =================================================================================
## input_8 (InputLayer)            [(None, 20)]                  0
## _________________________________________________________________________________
## dense_11 (Dense)                (None, 50)                    1050
## =================================================================================
## Total params: 1,050
## Trainable params: 1,050
```

```
## Non-trainable params: 0
## _________________________________________________________________________
```

```
aen_input2 = layer_input(shape = 50)
aen_output2 = aen_input2 %>%
  encoder2() %>%
  decoder2()

sae2 = keras_model(aen_input2, aen_output2)
summary(sae2)
```

```
## Model: "model_8"
## _________________________________________________________________________
## Layer (type)                 Output Shape              Param #
## =========================================================================
## input_9 (InputLayer)         [(None, 50)]              0
## _________________________________________________________________________
## model_6 (Model)              (None, 20)                1020
## _________________________________________________________________________
## model_7 (Model)              (None, 50)                1050
## =========================================================================
## Total params: 2,070
## Trainable params: 2,070
## Non-trainable params: 0
## _________________________________________________________________________
```

```
sae2 %>% compile(
  optimizer = "rmsprop",
  loss = "mse"
)
```

```
sae2 %>% fit(
  x=as.matrix(encoded_expression1),
  y=as.matrix(encoded_expression1),
  epochs = 25,
  batch_size=64,
  validation_split = 0.2
  )
```

```
#Generating with Autoencoder
encoded_expression2 <- encoder2 %>% predict(as.matrix(encoded_expression1))
```

AE3

```
input_enc3<-layer_input(shape = 20)
output_enc3<-input_enc3 %>%
  layer_dense(units=10,activation="relu")
encoder3 = keras_model(input_enc3, output_enc3)
summary(encoder3)
```

```
## Model: "model_9"
## _________________________________________________________________________
## Layer (type)                 Output Shape              Param #
## =========================================================================
## input_10 (InputLayer)        [(None, 20)]              0
## _________________________________________________________________________
```

```
## dense_12 (Dense)                    (None, 10)                    210
## ================================================================================
## Total params: 210
## Trainable params: 210
## Non-trainable params: 0
## ________________________________________________________________________________
```

```
input_dec3 = layer_input(shape = 10)
output_dec3<-input_dec3 %>%
  layer_dense(units=20,activation="linear")

decoder3 = keras_model(input_dec3, output_dec3)

summary(decoder3)
```

```
## Model: "model_10"
## ________________________________________________________________________________
## Layer (type)                        Output Shape                  Param #
## ================================================================================
## input_11 (InputLayer)               [(None, 10)]                  0
## ________________________________________________________________________________
## dense_13 (Dense)                    (None, 20)                    220
## ================================================================================
## Total params: 220
## Trainable params: 220
## Non-trainable params: 0
## ________________________________________________________________________________
```

```
aen_input3 = layer_input(shape = 20)
aen_output3 = aen_input3 %>%
  encoder3() %>%
  decoder3()

sae3 = keras_model(aen_input3, aen_output3)
summary(sae3)
```

```
## Model: "model_11"
## ________________________________________________________________________________
## Layer (type)                        Output Shape                  Param #
## ================================================================================
## input_12 (InputLayer)               [(None, 20)]                  0
## ________________________________________________________________________________
## model_9 (Model)                     (None, 10)                    210
## ________________________________________________________________________________
## model_10 (Model)                    (None, 20)                    220
## ================================================================================
## Total params: 430
## Trainable params: 430
## Non-trainable params: 0
## ________________________________________________________________________________
```

```
sae3 %>% compile(
  optimizer = "rmsprop",
  loss = "mse"
)
```

```
sae3 %>% fit(
  x=as.matrix(encoded_expression2),
  y=as.matrix(encoded_expression2),
  epochs = 25,
  batch_size=64,
  validation_split = 0.2
  )
```

```
#Generating with Autoencoder
encoded_expression3 <- encoder3 %>% predict(as.matrix(encoded_expression2))
```

Final model

```
sae_input = layer_input(shape = 142)
sae_output = sae_input %>%
  encoder1() %>%
  encoder2()  %>%
  encoder3() %>%
  layer_dense(5,activation = "relu")%>%
  layer_dense(1,activation = "sigmoid")

sae = keras_model(sae_input, sae_output)
summary(sae)
```

```
## Model: "model_12"
## _________________________________________________________________________________
## Layer (type)                         Output Shape                      Param #
## =================================================================================
## input_13 (InputLayer)                [(None, 142)]                     0
## _________________________________________________________________________________
## model_3 (Model)                      (None, 50)                        7150
## _________________________________________________________________________________
## model_6 (Model)                      (None, 20)                        1020
## _________________________________________________________________________________
## model_9 (Model)                      (None, 10)                        210
## _________________________________________________________________________________
## dense_15 (Dense)                     (None, 5)                         55
## _________________________________________________________________________________
## dense_14 (Dense)                     (None, 1)                         6
## =================================================================================
## Total params: 8,441
## Trainable params: 8,441
## Non-trainable params: 0
## _________________________________________________________________________________
```

```
freeze_weights(sae,from=1,to=3)
```

```
summary(sae)
```

```
## Model: "model_12"
## _________________________________________________________________________________
## Layer (type)                         Output Shape                      Param #
## =================================================================================
## input_13 (InputLayer)                [(None, 142)]                     0
## _________________________________________________________________________________
```

```
## model_3 (Model)                     (None, 50)                    7150
## ____________________________________________________________________________
## model_6 (Model)                     (None, 20)                    1020
## ____________________________________________________________________________
## model_9 (Model)                     (None, 10)                    210
## ____________________________________________________________________________
## dense_15 (Dense)                    (None, 5)                     55
## ____________________________________________________________________________
## dense_14 (Dense)                    (None, 1)                     6
## ============================================================================
## Total params: 8,441
## Trainable params: 271
## Non-trainable params: 8,170
## ____________________________________________________________________________
```

```
sae %>% compile(
  optimizer = "rmsprop",
  loss = 'binary_crossentropy',
  metric = "acc"
  )
```

```
sae %>% fit(
  x=xtrain,
  y=ylabels,
  epochs = 30,
  batch_size=64,
  validation_split = 0.2
  )
```

```
sae %>%
  evaluate(as.matrix(xtest), ytestlabels)
```

```
##      loss       acc
## 0.3607836 0.8281250
```

```
yhat <- predict(sae,as.matrix(xtest))
```

```
yhatclass<-as.factor(ifelse(yhat<0.5,0,1))
table(yhatclass,  ytestlabels)
```

```
##          ytestlabels
## yhatclass  0  1
##         0 13  2
##         1 20 93
```

```
confusionMatrix(yhatclass,as.factor(ytestlabels))
```

```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction  0  1
##          0 13  2
##          1 20 93
##
##                Accuracy : 0.8281
##                  95% CI : (0.7514, 0.889)
##     No Information Rate : 0.7422
```

```
##     P-Value [Acc > NIR] : 0.0142031
##
##                   Kappa : 0.4536
##
##  Mcnemar's Test P-Value : 0.0002896
##
##             Sensitivity : 0.3939
##             Specificity : 0.9789
##          Pos Pred Value : 0.8667
##          Neg Pred Value : 0.8230
##              Prevalence : 0.2578
##          Detection Rate : 0.1016
##    Detection Prevalence : 0.1172
##       Balanced Accuracy : 0.6864
##
##        'Positive' Class : 0
##
```

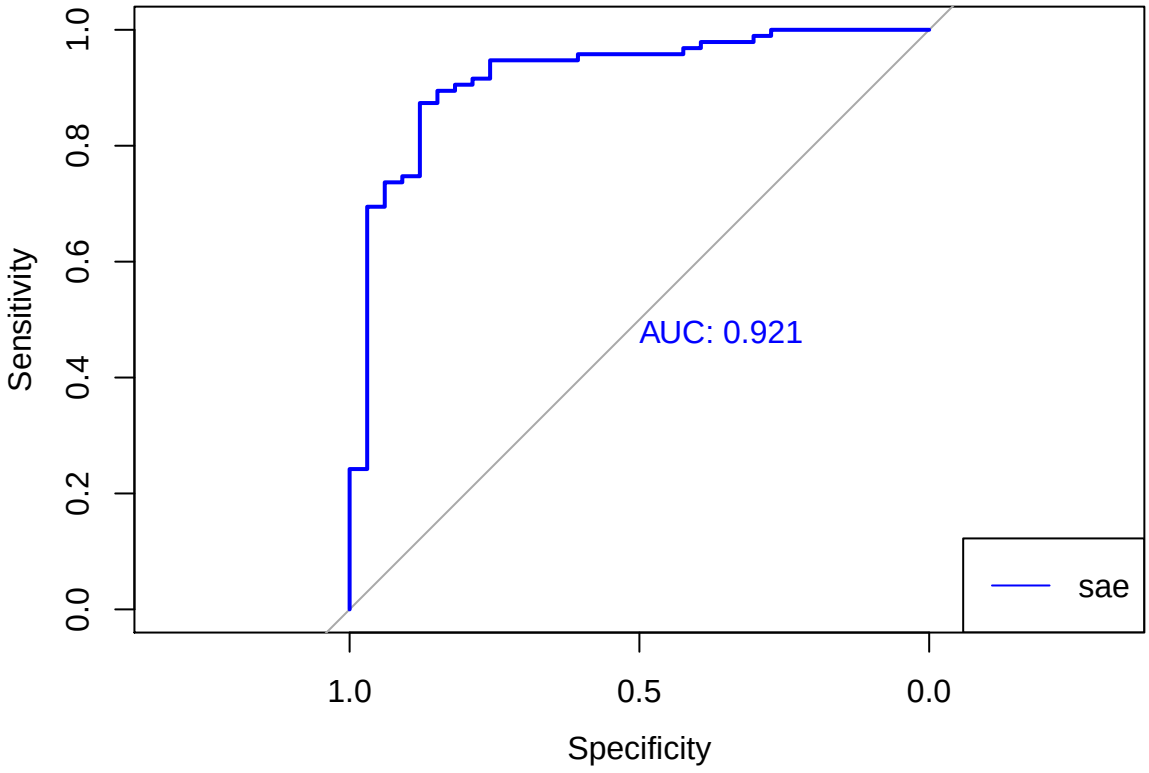
```
roc_sae_test <- roc(response = ytestlabels, predictor =yhat)
```

```
## Setting levels: control = 0, case = 1
```

```
## Warning in roc.default(response = ytestlabels, predictor = yhat): Deprecated use
## a matrix as predictor. Unexpected results may be produced, please pass a numeric
## vector.
```

```
## Setting direction: controls < cases
```

```
plot(roc_sae_test, col = "blue", print.auc=TRUE)
legend("bottomright", legend = c("sae"), lty = c(1), col = c("blue"))
```


Sensitivity
0.0
0.2
0.4
0.6
0.8
1.0
AUC: 0.921
sae
1.0
0.5
0.0
Specificity