

NeuralNetwork_Novikov

Vitalii Novikov

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Libraries

```
library <- function(...) {suppressPackageStartupMessages(base::library(...))}  
if (!require(caret)) install.packages("caret"); library(caret)
```

Loading required package: caret

Loading required package: ggplot2

Loading required package: lattice

```
if (!require(neuralnet)) install.packages("neuralnet"); library(neuralnet)
```

Loading required package: neuralnet

```
if (!require(mlbench)) install.packages("mlbench"); library(mlbench)
```

Loading required package: mlbench

```
if (!require(dplyr)) install.packages("dplyr"); library(dplyr)
```

Loading required package: dplyr

Attaching package: 'dplyr'

The following object is masked from 'package:neuralnet':

compute

The following objects are masked from 'package:stats':

filter, lag

The following objects are masked from 'package:base':

intersect, setdiff, setequal, union

```
library(plyr)
```

Starting point

We would like to use Neural Network to predict the diagnosis (Benign or Malignant based on 10 features: - radius (mean of distances from center to points on the perimeter) - texture (standard deviation of gray-scale values) - perimeter - area - smoothness (local variation in radius lengths) - compactness ($\text{perimeter}^2 / \text{area} - 1.0$) - concavity (severity of concave portions of the contour) - concave points (number of concave portions of the contour) - symmetry - fractal dimension ("coastline approximation" - 1)

Data management

First the data is collected from package "mlbench".

```
data("BreastCancer", package = "mlbench")
BreastCancer |> head()
```

	Id	Cl.thickness	Cell.size	Cell.shape	Marg.adhesion	Epith.c.size
1	1000025	5	1	1	1	2
2	1002945	5	4	4	5	7
3	1015425	3	1	1	1	2
4	1016277	6	8	8	1	3
5	1017023	4	1	1	3	2
6	1017122	8	10	10	8	7

	Bare.nuclei	Bl.cromatin	Normal.nucleoli	Mitoses	Class
1	1	3	1	1	benign
2	10	3	2	1	benign
3	2	3	1	1	benign
4	4	3	7	1	benign
5	1	3	1	1	benign
6	10	9	7	1	malignant

But it is wrong dataset.

Get another:

```
dat <- read.csv("data.csv")
glimpse(dat)
```

Columns: 33

```
nrow(dat)
```

This dataset include 569 observations. We will only use the “worst-features” for creating neural network.

Pick useful predictors

```
clean_data <- as_tibble(dat[c(2,23:32)])
clean_data <- mutate(clean_data,
  diagnosis = case_match(diagnosis, "M" ~ "malignant", "B"~ "benign")
) %>% mutate_if(is.character, as.factor)
#clean_data[['diagnosis']] <- as.factor(clean_data[['diagnosis']])
clean_data |> head(2)
```

```
# A tibble: 2 x 11
  diagnosis radius_worst texture_worst perimeter_worst area_worst
<fct>      <dbl>      <dbl>      <dbl>      <dbl>
1 malignant    25.4        17.3        185.        2019
2 malignant    25.0        23.4        159.        1956
# i 6 more variables: smoothness_worst <dbl>, compactness_worst <dbl>,
#   concavity_worst <dbl>, concave.points_worst <dbl>, symmetry_worst <dbl>,
#   fractal_dimension_worst <dbl>
```

```
clean_data |> apply(2, function(x) sum(is.na(x)))
```

diagnosis	radius_worst	texture_worst
0	0	0
perimeter_worst	area_worst	smoothness_worst
0	0	0
compactness_worst	concavity_worst	concave.points_worst
0	0	0
symmetry_worst	fractal_dimension_worst	
0	0	

There is no missing data, good.

Normalize the data

All predictors have their own scales. We should perform min-max-normalization.

```
clean_data |> summary()
```

diagnosis	radius_worst	texture_worst	perimeter_worst
benign :357	Min. : 7.93	Min. :12.02	Min. : 50.41
malignant:212	1st Qu.:13.01	1st Qu.:21.08	1st Qu.: 84.11
	Median :14.97	Median :25.41	Median : 97.66
	Mean :16.27	Mean :25.68	Mean :107.26
	3rd Qu.:18.79	3rd Qu.:29.72	3rd Qu.:125.40
	Max. :36.04	Max. :49.54	Max. :251.20

area_worst	smoothness_worst	compactness_worst	concavity_worst
Min. : 185.2	Min. :0.07117	Min. :0.02729	Min. :0.0000
1st Qu.: 515.3	1st Qu.:0.11660	1st Qu.:0.14720	1st Qu.:0.1145
Median : 686.5	Median :0.13130	Median :0.21190	Median :0.2267
Mean : 880.6	Mean :0.13237	Mean :0.25427	Mean :0.2722
3rd Qu.:1084.0	3rd Qu.:0.14600	3rd Qu.:0.33910	3rd Qu.:0.3829
Max. :4254.0	Max. :0.22260	Max. :1.05800	Max. :1.2520

concave.points_worst	symmetry_worst	fractal_dimension_worst
Min. :0.00000	Min. :0.1565	Min. :0.05504
1st Qu.:0.06493	1st Qu.:0.2504	1st Qu.:0.07146
Median :0.09993	Median :0.2822	Median :0.08004
Mean :0.11461	Mean :0.2901	Mean :0.08395
3rd Qu.:0.16140	3rd Qu.:0.3179	3rd Qu.:0.09208
Max. :0.29100	Max. :0.6638	Max. :0.20750

```

maxs <- apply(clean_data[-1], 2, max)
mins <- apply(clean_data[-1], 2, min)

scaled_data <- scale(clean_data[-1], center = mins, scale = maxs - mins) %>%
  cbind(clean_data[1])

summary(scaled_data)

```

radius_worst	texture_worst	perimeter_worst	area_worst
Min. :0.0000	Min. :0.0000	Min. :0.0000	Min. :0.00000
1st Qu.:0.1807	1st Qu.:0.2415	1st Qu.:0.1678	1st Qu.:0.08113
Median :0.2504	Median :0.3569	Median :0.2353	Median :0.12321
Mean :0.2967	Mean :0.3640	Mean :0.2831	Mean :0.17091
3rd Qu.:0.3863	3rd Qu.:0.4717	3rd Qu.:0.3735	3rd Qu.:0.22090
Max. :1.0000	Max. :1.0000	Max. :1.0000	Max. :1.00000

smoothness_worst	compactness_worst	concavity_worst	concave.points_worst
Min. :0.0000	Min. :0.0000	Min. :0.00000	Min. :0.0000
1st Qu.:0.3000	1st Qu.:0.1163	1st Qu.:0.09145	1st Qu.:0.2231
Median :0.3971	Median :0.1791	Median :0.18107	Median :0.3434
Mean :0.4041	Mean :0.2202	Mean :0.21740	Mean :0.3938

3rd Qu.:0.4942	3rd Qu.:0.3025	3rd Qu.:0.30583	3rd Qu.:0.5546
Max. :1.0000	Max. :1.0000	Max. :1.00000	Max. :1.0000
symmetry_worst	fractal_dimension_worst	diagnosis	
Min. :0.0000	Min. :0.0000	benign :357	
1st Qu.:0.1851	1st Qu.:0.1077	malignant:212	
Median :0.2478	Median :0.1640		
Mean :0.2633	Mean :0.1896		
3rd Qu.:0.3182	3rd Qu.:0.2429		
Max. :1.0000	Max. :1.0000		

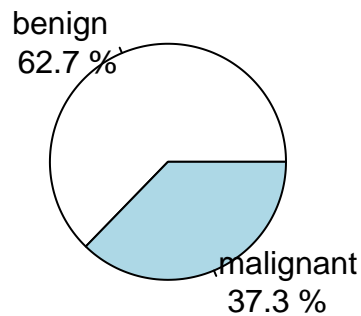
Now we have all predictors in the same scale.

Balance of the data

```
#custom function to create pie chart
pie_with_percentages <- function(diag_list, main = "Diagnosis", round = 1) {
  diag_table <- table(diag_list)
  diag_percentages <- prop.table(diag_table) * 100
  labels <- paste(names(diag_table), "\n", round(diag_percentages, round), "%")
  return(pie(diag_table, labels = labels, main = main))
}

pie_with_percentages(scaled_data$diagnosis)
```

Diagnosis



Our dataset do not show the perfect balance of diagnosis, but it is still not that bad as 90/10 or 99/1 split. Neural networks, by default, tend to favor the majority class. This means the model might become biased towards predicting “benign,” potentially leading to poor performance in identifying “malignant” cases.

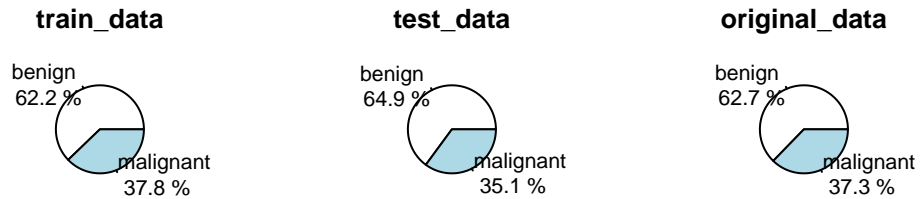
In the next step stratified data set will be created to minimize the potential bias.

Stratified data set

Using ‘sample’ function

```
set.seed(230)
index <- sample(1:nrow(scaled_data), round(0.8*nrow(scaled_data)))
train_data <- scaled_data[index,]
test_data <- scaled_data[-index,]

layout(matrix(c(1,2,3), nrow = 1), respect = TRUE)
pie_with_percentages(train_data$diagnosis, main = "train_data")
pie_with_percentages(test_data$diagnosis, main = "test_data")
pie_with_percentages(clean_data$diagnosis, main = "original_data")
```

```
layout(1)
```

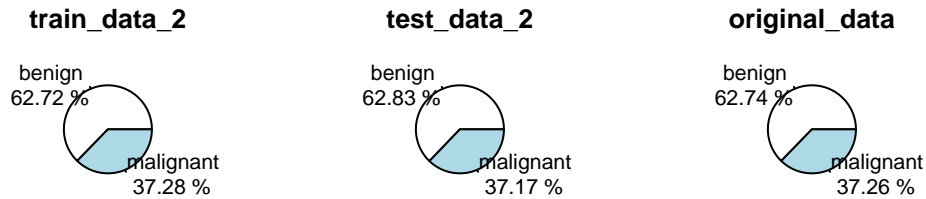
The test data show slightly lowest proportion of malignant then both train and original data, but it is still very close to actual picture.

Using caret library

```
set.seed(123)
index_2 <- createDataPartition(scaled_data$diagnosis, p = 0.8, list = FALSE)

train_data_2 <- scaled_data[index_2,]
test_data_2 <- scaled_data[-index_2,]

layout(matrix(c(1,2,3), nrow = 1), respect = TRUE)
pie_with_percentages(train_data_2$diagnosis, main = "train_data_2", round = 2)
pie_with_percentages(test_data_2$diagnosis, main = "test_data_2", round = 2)
pie_with_percentages(clean_data$diagnosis, main = "original_data", round = 2)
```



In this case we got really stratified train and test split of the data, because the proportions of classes are almost the same in each dataset. For further steps we will use this split of the data.

```
trainD <- train_data_2
testD <- test_data_2

split_description <- t(rbind(
  data.frame("trainD" = nrow(trainD), "testD" = nrow(testD)),
  c(round(nrow(trainD)/nrow(clean_data)*100,2),
    round(nrow(testD)/nrow(clean_data)*100,2))
))
colnames(split_description) <- c("nrow","percentage (%)")
split_description
```

	nrow	percentage (%)
trainD	456	80.14
testD	113	19.86

The trainD include 456 rows, which is 80.14% of the original dataset.

Hyperparameters tuning

First NN

```
set.seed(1)
model1 <- neuralnet(diagnosis ~ . , data = trainD, hidden = c(5,3), linear.output=FALSE)
plot(model1)
```

As an example of NN the model with 2 hidden layers (with 5 and 3 neurons) were created. The black lines show the connections between each layer and the weights on each connection while the blue lines show the bias term added in each step.

Model evaluation

The most interesting thing to explore after creating classification model is confusion matrix. But in this step the real test data were used to evaluate the model. For further steps the validation data will be created.

```
pred <- neuralnet::compute(model1, testD[, -11])$net.result

labels <- c("benign", "malignant")
prediction_label <- (data.frame(max.col(pred)) %>%
  mutate(pred=labels[max.col(pred.)]))[2] %>%
  unlist()

table(testD$diagnosis, prediction_label)
```

	prediction_label	
	benign	malignant
benign	69	2
malignant	2	40

The confusion matrix shows that the model made 4 mistakes.

```
check = as.numeric(testD$diagnosis) == max.col(pred)
accuracy = (sum(check)/nrow(testD))*100
print(accuracy)
```

```
[1] 96.46018
```

Therefore the accuracy is about 96.5%.

But we would like to use **cross-entropy** as the error function. There is no ready-to-use *cross-entropy loss* function in neuralnet, therefore we should calculate loss manually.

```
true_one_hot <- testD["diagnosis"] %>%  
  mutate(diagnosis = case_match(diagnosis,  
    "malignant" ~ 0,  
    "benign" ~ 1  
  ))  
  
cross_entropy <- -sum(true_one_hot * log(pred)) / nrow(testD)  
cross_entropy
```

```
[1] 0.3530022
```

It is hard to interpret this number, because it is not a direct loss function like RSME. But we would like to minimize Cross Entropy when compare models.

Change hidden level parameters

First, the 5 fold stratified data split is created.

```
set.seed(321)  
folds <- createFolds(trainD$diagnosis, k = 5, list = TRUE, returnTrain = FALSE)  
  
possible_levels <- c(1,2)  
possible_neurons <- 2:5  
validation_table <- data.frame(hidden_levels=integer(0),  
  l1_neurons=integer(0),  
  l2_neurons=integer(0),  
  ce1=numeric(0),  
  ce2=numeric(0),  
  ce3=numeric(0),  
  ce4=numeric(0),  
  ce5=numeric(0),  
  cross_entropy_avg=numeric(0),  
  accuracy_avg=numeric(0))  
  
# 1 hidden level loop  
for(n in possible_neurons){
```

```

accuracy_list = numeric(0)
cross_entropy_list = numeric(0)
for(i in 1:5) {
  test_index <- folds[[i]]
  train_fold <- trainD[-test_index, ]
  test_fold <- trainD[test_index, ]
  set.seed(5)
  model_nn <- neuralnet(diagnosis ~ . , data = train_fold, hidden = n, linear.output=FALSE)
  pred <- neuralnet::compute(model_nn, test_fold[, -11])$net.result
  #ce
  true_one_hot <- test_fold["diagnosis"] %>%
  mutate(diagnosis = case_match(diagnosis,
    "malignant" ~ 0,
    "benign" ~ 1
  ))
  cross_entropy_list[i] <- -sum(true_one_hot * log(pred)) / nrow(test_fold)
  #ac
  check = as.numeric(test_fold$diagnosis) == max.col(pred)
  accuracy_list[i] <- (sum(check)/nrow(test_fold))*100
}
validation_table[nrow(validation_table) + 1, ] <- c(1, n, NA,
                                                    cross_entropy_list,
                                                    mean(cross_entropy_list),
                                                    mean(accuracy))
}
# 2 hidden levels loop
for(n1 in possible_neurons){
  for(n2 in possible_neurons){
    accuracy_list = numeric(0)
    cross_entropy_list = numeric(0)
    for(i in 1:5) {
      test_index <- folds[[i]]
      train_fold <- trainD[-test_index, ]
      test_fold <- trainD[test_index, ]
      set.seed(5)
      model_nn <- neuralnet(diagnosis ~ . , data = train_fold, hidden = c(n1,n2), linear.outp
      pred <- neuralnet::compute(model_nn, test_fold[, -11])$net.result
      #ce
      true_one_hot <- test_fold["diagnosis"] %>%
      mutate(diagnosis = case_match(diagnosis,
        "malignant" ~ 0,
        "benign" ~ 1

```

```

))
cross_entropy_list[i] <- -sum(true_one_hot * log(pred)) / nrow(test_fold)
#ac
check = as.numeric(test_fold$diagnosis) == max.col(pred)
accuracy_list[i] = (sum(check)/nrow(test_fold))*100
}
validation_table[nrow(validation_table) + 1, ] <- c(2, n1, n2,
                                                    cross_entropy_list,
                                                    mean(cross_entropy_list),
                                                    mean(accuracy_list))
}
}

apply(validation_table,2 ,function(x) round(x,2))

```

	hidden_levels	l1_neurons	l2_neurons	ce1	ce2	ce3	ce4	ce5
1		1	2	NA	0.38	0.50	0.09	0 0.09
2		1	3	NA	0.16	0.36	0.07	0 0.15
3		1	4	NA	0.19	0.45	0.04	0 0.00
4		1	5	NA	0.17	0.34	0.12	0 0.01
5		2	2	2	0.16	0.11	0.05	0 0.00
6		2	2	3	0.12	0.49	0.05	0 0.12
7		2	2	4	0.15	0.64	0.10	0 0.00
8		2	2	5	0.23	0.11	0.04	0 0.04
9		2	3	2	0.13	1.48	0.13	0 0.05
10		2	3	3	0.00	1.10	0.12	0 0.05
11		2	3	4	0.22	0.50	0.02	0 0.18
12		2	3	5	0.30	0.51	0.13	0 0.00
13		2	4	2	0.03	0.06	0.01	0 0.11
14		2	4	3	0.13	0.27	0.04	0 0.07
15		2	4	4	0.00	0.07	0.05	0 0.04
16		2	4	5	0.21	0.50	0.02	0 0.07
17		2	5	2	0.17	0.07	0.02	0 0.11
18		2	5	3	0.04	0.21	0.08	0 0.15
19		2	5	4	0.12	0.54	0.11	0 0.05
20		2	5	5	0.03	0.32	0.08	0 0.08
	cross_entropy_avg	accuracy_avg						
1		0.21	96.46					
2		0.15	96.46					
3		0.14	96.46					
4		0.13	96.46					
5		0.07	96.93					

6	0.16	96.27
7	0.18	96.93
8	0.08	96.93
9	0.36	96.27
10	0.25	96.71
11	0.19	97.37
12	0.19	96.27
13	0.04	96.49
14	0.10	97.37
15	0.03	96.05
16	0.16	96.93
17	0.07	96.93
18	0.10	96.49
19	0.16	96.49
20	0.10	96.71

Somehow cross entropy for the 4th fold is 0

Recheck it:

```
validation_table$ce4
```

```
[1] 2.550464e-05 2.147966e-05 1.177995e-05 9.935263e-06 5.066267e-06
[6] 4.548479e-06 3.116685e-06 3.684743e-06 2.777155e-05 5.998682e-04
[11] 9.903698e-07 6.941158e-06 1.408572e-05 7.800080e-06 5.397184e-06
[16] 3.366158e-06 4.751372e-05 1.712628e-05 3.386463e-06 2.708440e-06
```

It is not 0 in most cases, but very close to zero.

```
vt <- validation_table %>% mutate(
  node = case_when(
    hidden_levels==1 ~ paste0("(",l1_neurons,")"),
    hidden_levels==2 ~ paste0("(",l1_neurons,",",l2_neurons,")")
  )
)
vt$node <- factor(vt$node, levels = vt$node)
vt[c("node", "cross_entropy_avg", "accuracy_avg")] %>%
  sort_by(vt$cross_entropy_avg) %>%
  head() %>% knitr::kable()
```

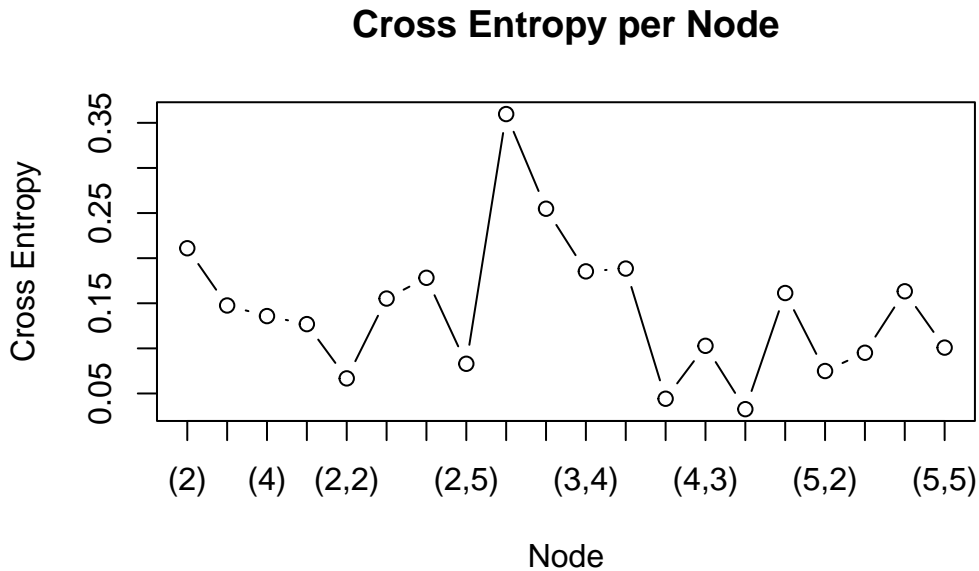
	node	cross_entropy_avg	accuracy_avg
15	(4,4)	0.0326244	96.05351
13	(4,2)	0.0442029	96.49307
5	(2,2)	0.0667386	96.93024
17	(5,2)	0.0749148	96.93263
8	(2,5)	0.0829441	96.93024
18	(5,3)	0.0951407	96.49068

This table represents lowest cross_entropy_avg for models.

The neural network with hyperparameters (4,4) shows the lowest cross entropy loss. This model will be used for further steps.

```
plot(1:length(vt$node), vt$cross_entropy_avg, type = "b",
     xlab = "Node", ylab = "Cross Entropy",
     main = "Cross Entropy per Node", xaxt = "n")

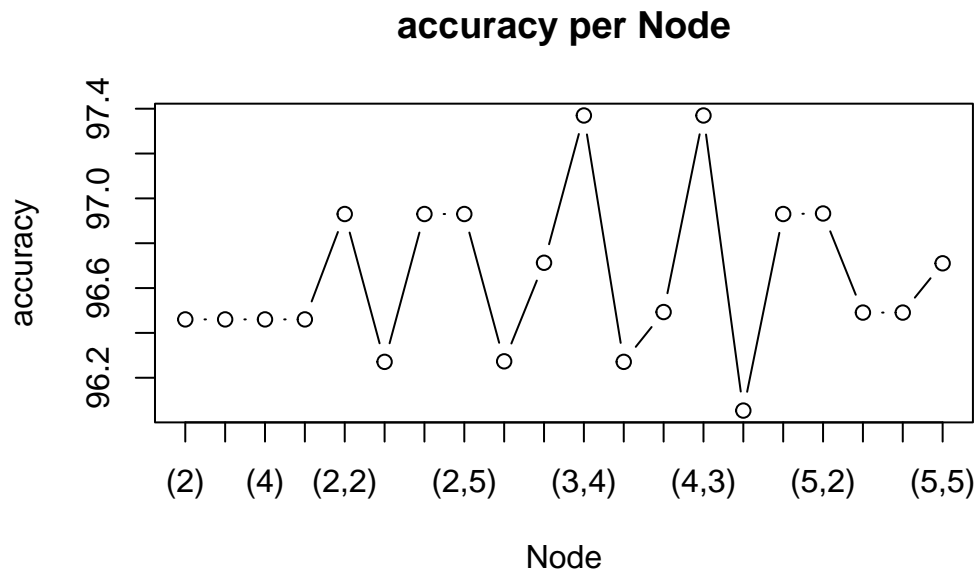
axis(1, at = 1:length(vt$node), labels = vt$node)
```



There is no special pattern in cross_entropy_avg when the number of neurons increases.

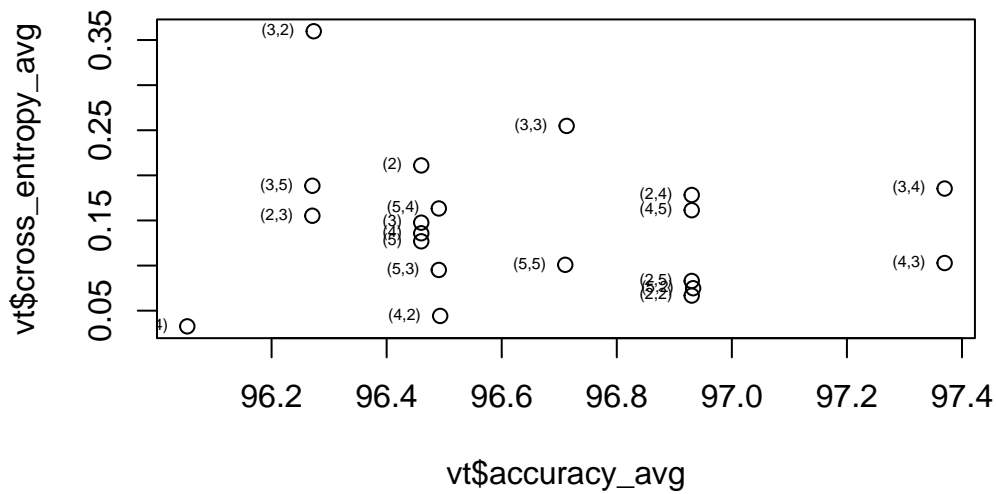

```
plot(1:length(vt$node), vt$accuracy_avg, type = "b",
     xlab = "Node", ylab = "accuracy",
     main = "accuracy per Node", xaxt = "n")

axis(1, at = 1:length(vt$node), labels = vt$node)
```



The accuracy fluctuates between 96 and 97 in most cases, but for (3,4) and (4,3) it becomes larger than 97, whereas (4,4) nn shows the lowest accuracy within networks (96.05).

```
plot(x=vt$accuracy_avg, y=vt$cross_entropy_avg)
text(x = vt$accuracy_avg, y = vt$cross_entropy_avg, labels = vt$node, pos = 2, cex = 0.5)
```



Another possible neural network, that could be good choice for using is nn with 2 hidden layers and (4,3) neurons on these layers, because it is the closest to right bottom corner, which means that the model shows good balance of accuracy and loss function.

But we would like to choose the model with the lowest cross entropy loss, so the (4,4) is a winning model.

Final model

Train & test model

Now the whole trainD set is used for training.

```
set.seed(2)
nn <- neuralnet(diagnosis ~ . , data = testD, hidden = c(4,4), linear.output=FALSE)
pred <- neuralnet::compute(nn, testD[, -11])$net.result
#ce
true_one_hot <- testD["diagnosis"] %>%
mutate(diagnosis = case_match(diagnosis,
  "malignant" ~ 0,
  "benign" ~ 1
))
```

```

cross_entropy <- -sum(true_one_hot * log(pred)) / nrow(testD)
#ac
check = as.numeric(testD$diagnosis) == max.col(pred)
accuracy = (sum(check)/nrow(testD))*100

# confusion matrix
labels <- c("benign", "malignant")
prediction_label <- (data.frame(max.col(pred)) %>%
  mutate(pred=labels[max.col.pred.]))[2] %>%
  unlist()

table(testD$diagnosis, prediction_label)

```

	prediction_label	
	benign	malignant
benign	71	0
malignant	0	42

The confusion matrix shows that the model performed with flying colors, because there is no false negative and false positive predictions

```
print(paste0("Accuracy: ",accuracy,"%"))
```

```
[1] "Accuracy: 100%"
```

```
print(paste0("Cross Entropy: ",round(cross_entropy,4)))
```

```
[1] "Cross Entropy: 0.0013"
```

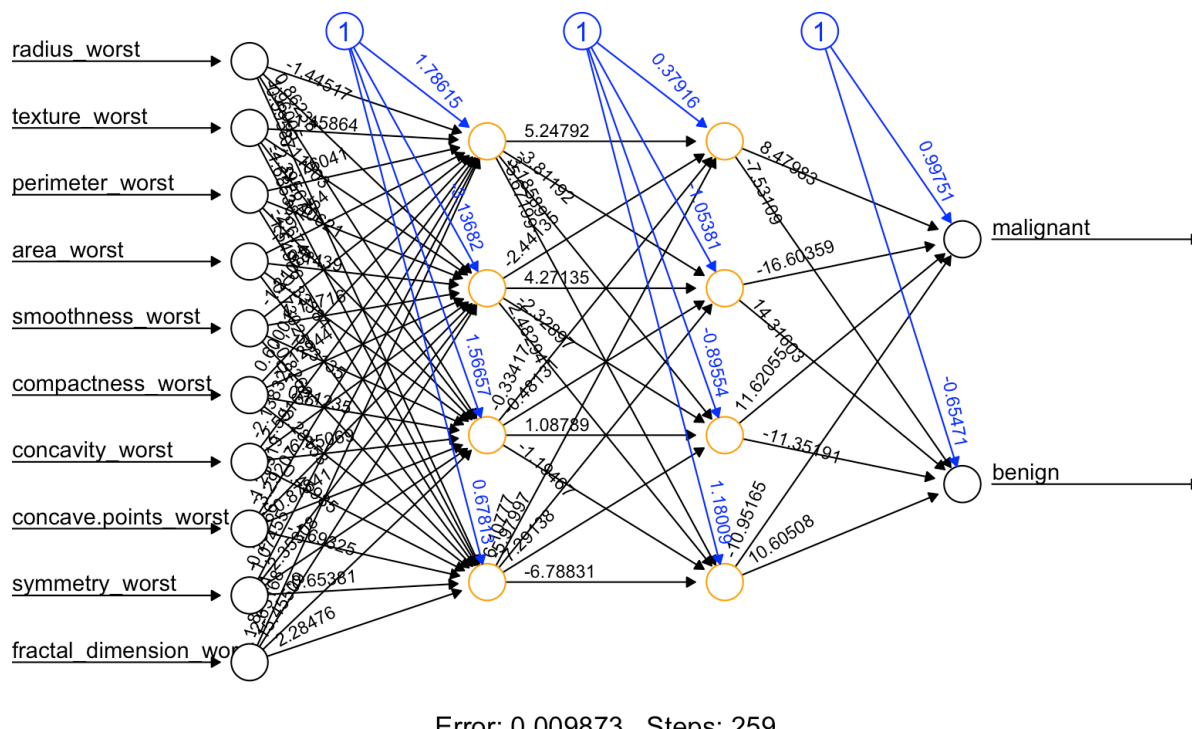
So, the accuracy is 100%, while the loss is very comparing to models that were on previous steps.

Model vizualization

```

png("neuralnet_plot.png")
plot(nn, col.hidden = "orange", fontsize = 10, information.pos = 0.25)
knitr::include_graphics("neuralnet_plot.png")

```



The black lines show the connections between each layer and the weights on each connection, while the blue lines show the bias term added at each step. The black neurons on the left are inputs, and the black neurons on the right are outputs. Orange neurons are part of the hidden layers.

Problem of overfitting

Overfitting means a neural network performs well on training data, poorly on unseen data. It memorizes, not generalizes. The detection of it can be via comparing training and validation performance, because a large gap between them indicates overfitting. Some ways to prevent overfitting: - Early stopping (of course with monitoring validation loss) - Regularization (L1/L2), but it reduces model complexity - Dropping randomly disables neurons - Expanding the dataset to enhance the variety of training data.

There is no problem with overfitting in the final model, but sometimes neural networks tend to be overfitted especially if the data is not balanced. In this case the balance of resulting class is 37/63, which is not so bad. Also we used stratified split to perform as good as possible.