Solution 1: Multiclass and Softmax Regression

(a) Read in the MNIST data set

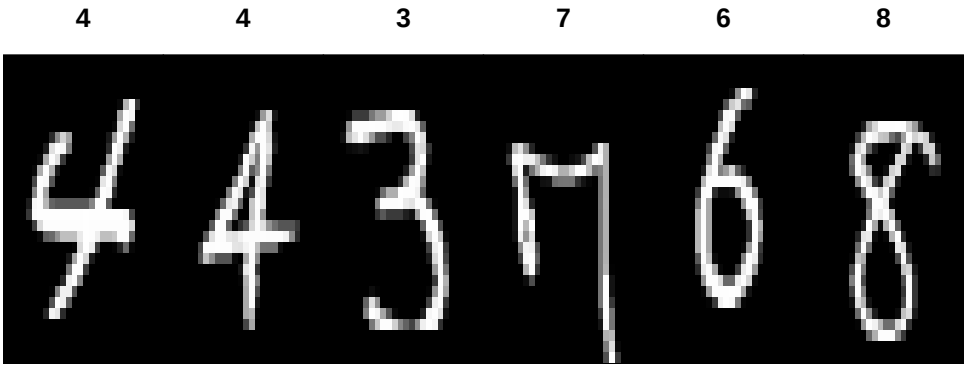
```
library(keras)
mnist <- dataset_mnist()

## Loaded Tensorflow version 2.8.1
```

(b) Visualize the data like

```
library(keras)
mnist <- dataset_mnist()
x_train <- mnist$train$x
y_train <- mnist$train$y
x_test <- mnist$test$x
y_test <- mnist$test$y

# visualize the digits
par(mfcol=c(1,6))
par(mar=c(0, 0, 3, 0), xaxs='i', yaxs='i')
for (idx in sample(1:NROW(x_train), 6)) {
    im <- x_train[idx,,]
    im <- t(apply(im, 2, rev))
    image(1:28, 1:28, im, col=gray((0:255)/255),
          xaxt='n', main=paste(y_train[idx]),
          yaxt='n')
}
```



(c) Convert the features to a (`pandas`) data frame, by flattening the 28x28 images to a 784-entry-long vector, which represents one row in your data frame. Divide the intensity values of each pixel (each column) by 255 to get a value between 0 and 1.

```
library(tibble)
# reshape
dim(x_train) <- c(nrow(x_train), 784)
dim(x_test) <- c(nrow(x_test), 784)
```

```
# rescale
x_train <- x_train / 255
x_test <- x_test / 255
# convert to data.frame
x_train <- as_tibble(as.data.frame(x_train))
x_test <- as_tibble(as.data.frame(x_test))
```

(d) Softmax regression

```
library(nnet)
data <- cbind(y = as.factor(y_train), x_train)
# note: takes some time and requires quite some memory
# also you need to set the maximum number of weights to get it running
# we will further restrict the maximum number of iterations
# to avoid overfitting (explanation is given later)
model <- multinom(y ~ -1 + ., data = data, MaxNWts = 7860, maxit = 20)
```

```
## # weights:  7850 (7056 variable)
## initial  value 138155.105580
## iter  10 value 30790.232712
## iter  20 value 23682.853837
## final  value 23682.853837
## stopped after 20 iterations
```

Look at the larger weights:

```
summary(model$wts)
```

```
##      Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
## -0.754937 -0.036317  0.000000 -0.003706  0.009061  0.842105
```

```
which.max(abs(model$wts))
```

```
## [1] 1192
```

```
dim(coef(model))
```

```
## [1]   9 784
```

There seem to be a few very large coefficients

(e) Use `keras`:

```
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
## The following objects are masked from 'package:stats':
##
##     filter, lag
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(keras)

# convert outcome using one-hot encoding
y_train_one_hot <- to_categorical(y_train)
y_test_one_hot <- to_categorical(y_test)

neural_network <- keras_model_sequential()

neural_network %>%
  layer_dense(units = 10, # corresponding to the number of classes
              activation = "softmax",
              input_shape = list(784)) %>%
  compile(
    optimizer = "adam",
    loss      = "categorical_crossentropy",
    metric = "accuracy"
  )

history_minibatches <- fit(
  object           = neural_network,
  x                = as.matrix(x_train),
  y                = y_train_one_hot,
  batch_size       = 24,
  epochs           = 80,
  validation_split = 0.2,
  callbacks = list(callback_early_stopping(patience = 10)),
  verbose = FALSE, # set this to TRUE to get console output
  view_metrics = FALSE # set this to TRUE to get a dynamic graphic output in RStudio
)
```

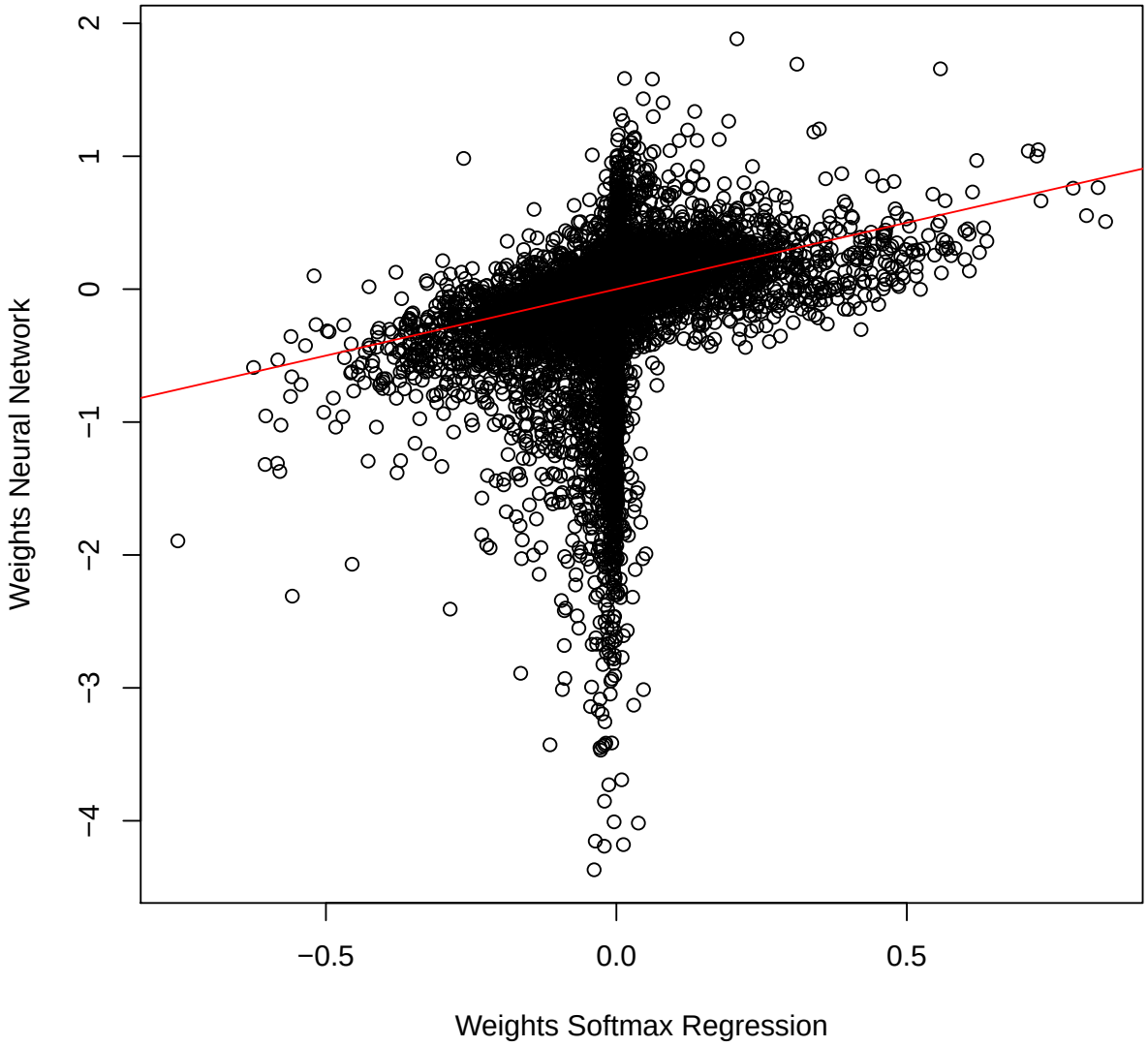
Look at the network weights

```
library(tensorflow)
tensor_weights <- as.matrix(tf$add(neural_network$weights[[1]],0))
summary(c(tensor_weights))

##      Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
## -4.36835 -0.45000 -0.07435 -0.23167  0.08794  1.88367
```

and compare to the ones from multinomial logistic regression:

```
plot(c(tensor_weights[,-1]) ~ c(t(coef(model))),
     xlab = "Weights Softmax Regression", ylab = "Weights Neural Network")
abline(0,1, col="red")
```



As both models de facto are based on neural networks (here the implementation of the softmax regression is actually done by fitting a neural network with the very same network structure), their similarity depends on how the network is trained. While clearly the implementation calling Python with backend `TensorFlow` (the `keras` fit) is much much faster, the network also converges more quickly due to a small batch size while the multinomial logistic regression calls a network fitting algorithm that uses batch size equal to the number of observations (which is usually a bad idea).

(f) First define the metrics

```r
# Classification error (how many of the predictions are wrong)
classiferror <- function(actual, predicted) {
    return(mean(actual != predicted))
}

# Accuracy (how many of the predictions are correct)
accuracy <- function(actual, predicted) {
    return(1 - classiferror(actual, predicted))
}
```

```r
# As we will usually have probabilistic predictions,
# we need to convert those to classes for the above
# metrics using the class with the max probability
probs_to_class <- function(probvec) {
  which.max(probvec)-1
}

#' MC Brier score
mcbrier <- function(actual_one_hot, prob) {
  rowSums((actual_one_hot-prob)^2)
}

# Cross-Entropy loss
crossentropy <- function(actual_one_hot, prob) {
  rowSums( -log(prob) * actual_one_hot )
}

# negative log-likelihood of multinomial distribution
loglikmultinom <- function(actual_one_hot, prob) {
  sapply(1:nrow(actual_one_hot), function(i)
    dmultinom(actual_one_hot[i,],
              size = 1, prob[i,], log = TRUE))
}
```

Now we get the predictions:

```r
pred_multinom <- predict(model, x_test, type = "probs")
pred_nn <- predict(neural_network, as.matrix(x_test))
str(pred_multinom, 1)

##  num [1:10000, 1:10] 0.001922 0.019599 0.000202 0.98602 0.00456 ...
##  - attr(*, "dimnames")=List of 2

str(pred_nn, 1)

##  num [1:10000, 1:10] 1.56e-08 2.15e-05 5.14e-07 1.00 3.16e-04 ...
```

Let's first look at the confusion matrix (in this case for the multinomial regression):

```r
table(y_test, apply(pred_multinom,1,probs_to_class))

##
## y_test    0    1    2    3    4    5    6    7    8    9
##      0  904    0    0    3    1   55   12    2    3    0
##      1    0 1108    2   10    1    1    5    2    6    0
##      2    8   11  874   34    9    6   20   15   47    8
##      3    6    0   11  926    3   15    5    9   26    9
##      4    0    5    2    4  901    2   13    4    3   48
##      5   11    1    3   54   13  703   23   10   62   12
##      6    9    3    4    1    8   16  913    2    2    0
##      7    4   14    9   11    8    1    1  938    3   39
##      8   10   14    5   48   12   22   16   12  813   22
##      9    8    5    1   19   41    6    1   19    7  902
```

Now the metrics. Classification error:

```
cbind(multinom = classiferror(y_test, apply(pred_multinom,1,probs_to_class)),
      neural = classiferror(y_test, apply(pred_nn,1,probs_to_class))
)

##      multinom neural
## [1,]   0.1018 0.0723
```

Accuracy:

```
cbind(multinom = accuracy(y_test, apply(pred_multinom,1,probs_to_class)),
      neural = accuracy(y_test, apply(pred_nn,1,probs_to_class))
)

##      multinom neural
## [1,]   0.8982 0.9277
```

MC Brier score (note that we look at the mean, because the definition of the loss is on an observation basis):

```
cbind(multinom = mean(mcbrier(y_test_one_hot, pred_multinom)),
      neural = mean(mcbrier(y_test_one_hot, pred_nn))
)

##       multinom    neural
## [1,] 0.1658749 0.1119277
```

Cross-entropy (mean):

```
cbind(multinom = mean(crossentropy(y_test_one_hot, pred_multinom)),
      neural = mean(crossentropy(y_test_one_hot, pred_nn))
)

##      multinom    neural
## [1,] 0.383929 0.2705714
```

Mean negative log-likelihood of multinomial distribution:

```
cbind(multinom = mean(loglikmultinom(y_test_one_hot, pred_multinom)),
      neural = mean(loglikmultinom(y_test_one_hot, pred_nn))
)

##       multinom     neural
## [1,] -0.383929 -0.2705714
```