Solution 1:

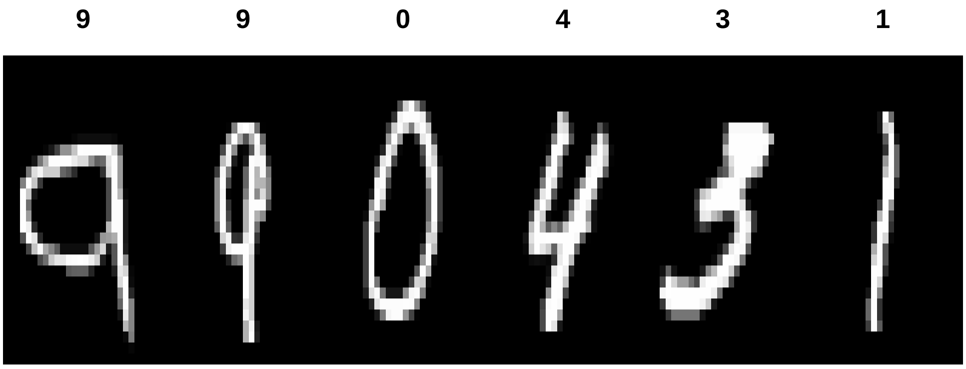
(a) Read in the MNIST data set

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

(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`:

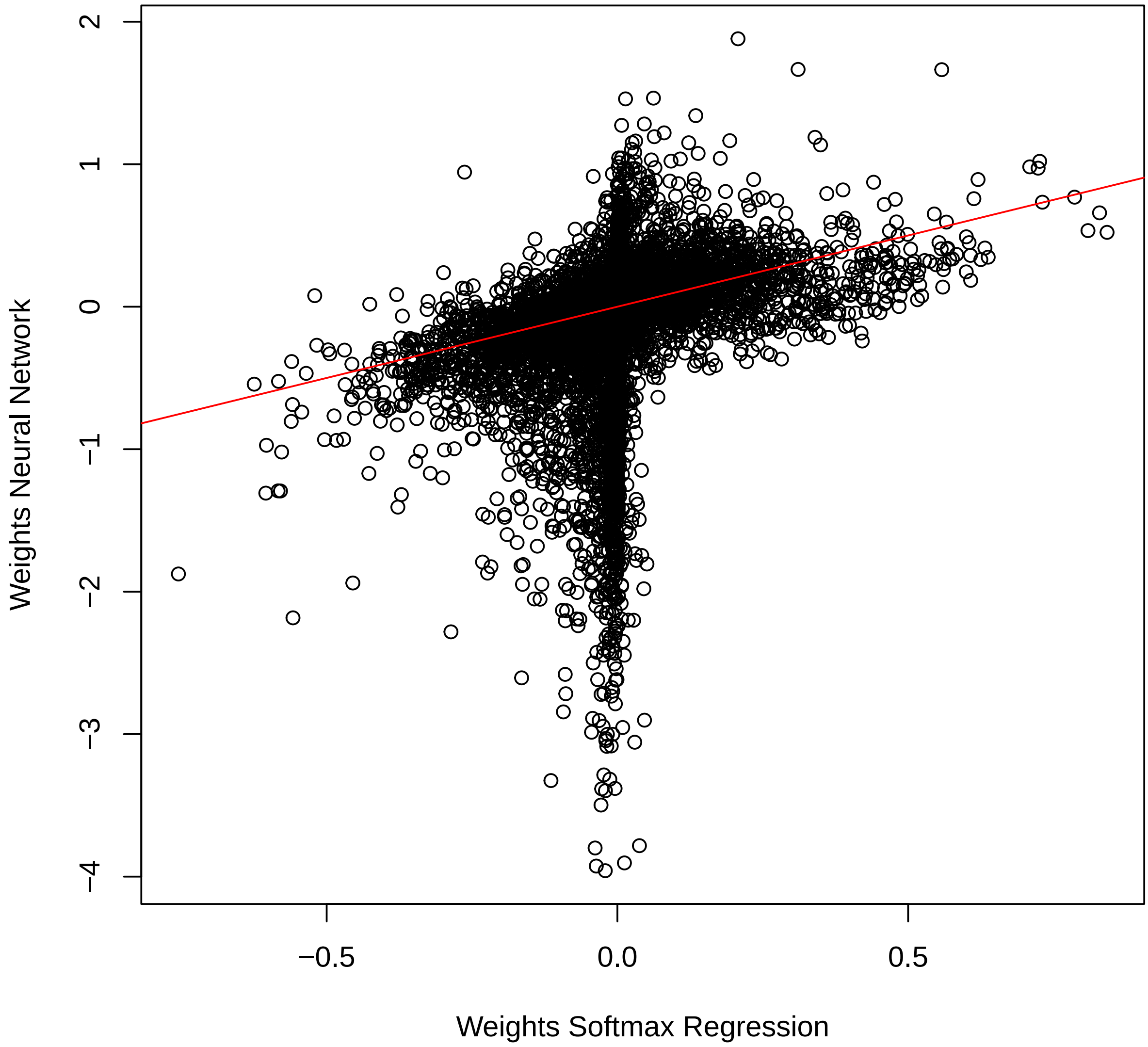
Look at the network weights

```
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.
## -3.95841 -0.43802 -0.07607 -0.21903  0.08510  1.88038
```

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 logisitic 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

```
# 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] 2.65e-08 2.08e-05 4.80e-07 1.00 3.20e-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 0.0739
```

Accuracy:

```
# Classification error
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 0.9261
```

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 0.1139504
```

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 0.2757474
```

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 -0.2757474
```

Solution 2:

(a) The logistic function is a special case of the softmax for two classes. We have

$$\pi_1(x) = \frac{\exp(\theta_1^\top x)}{\exp(\theta_1^\top x) + \exp(\theta_2^\top x)}$$

and

$$\pi_2(x) = \frac{\exp(\theta_2^\top x)}{\exp(\theta_1^\top x) + \exp(\theta_2^\top x)}.$$

We get:

$$\pi_1(x) = \frac{1}{(\exp(\theta_1^\top x) + \exp(\theta_2^\top x))/\exp(\theta_1^\top x)} = \frac{1}{\exp((\theta_1 - \theta_1)^\top x) + \exp((\theta_2 - \theta_1)^\top x)} = \frac{1}{1 + \exp(\theta^\top x)}$$

where $\theta = \theta_2 - \theta_1$ and $\pi_2(x) = 1 - \pi_1(x)$.

(b) For g classes and $n = 1$ trials (actually we are dealing with a multinoulli or categorial distribution), the likelihood $l(\boldsymbol{\pi})$ of a single observation y is given by

$$l(\boldsymbol{\pi}) = \prod_{k=1}^{g} \pi_k^{\mathbb{1}_{\{y=k\}}}.$$

Now let's look at the logarithmic loss in softmax regression:

$$\text{MC logloss} = -\sum_{k=1}^{g} \mathbb{1}_{\{y=k\}} \log \pi_k.$$

This is in fact just the negative logarithm of our likelihood: $-\log l(\boldsymbol{\pi}) = -\sum_{k=1}^{g} \mathbb{1}_{\{y=k\}} \log \pi_k$.