Statistical Learning (5454) - Assignment 4

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Exercise 1

We generate data from the additive error model $Y = f(X_1, X_2) + \epsilon$, where $f(X_1, X_2)$ is a sum of sigmoids, i.e.

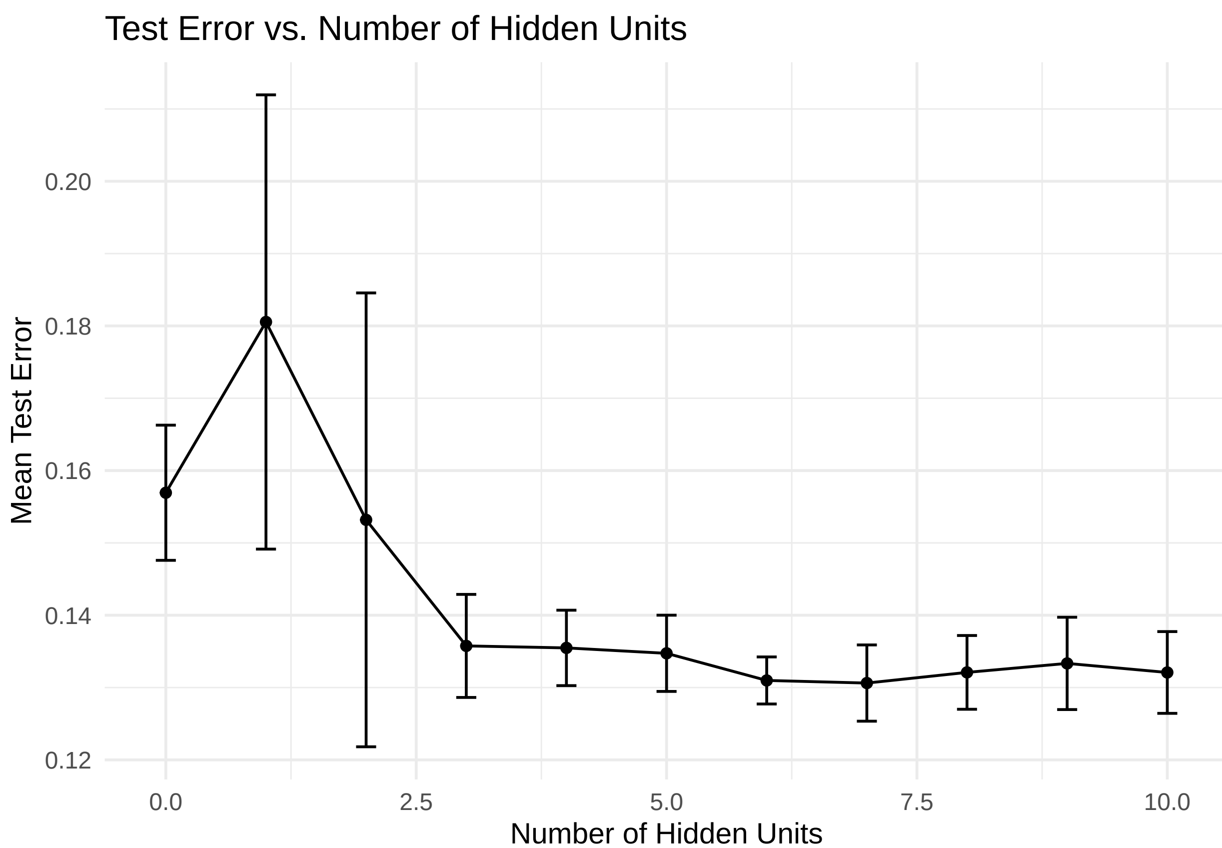
$$f(X_1, X_2) = \sigma(a_1^\top X_1) + \sigma(a_2^\top X_2),$$

with $a_1 = (3, 3)'$, $a_2 = (3, -3)'$ and bivariate standard Gaussian variables X_j, $j = 1, 2$. The variance of the independent Gaussian error ϵ is chosen such that the signal-to-noise ratio as measured by the respective variances equals four. We generate a training set of size 100 and a test sample of size 10,000.

We then fit neural networks with weight decay of 0.0005 and vary the number of hidden units from 0 to 10. We record the average test error $E_{\text{Test}}(Y - \hat{f}(X_1, X_2))^2$ for each of 10 random starting weights.

```
##    hidden_units mean_test_error sd_test_error
## 1             0       0.1569335   0.009344669
## 2             1       0.1805459   0.031403812
## 3             2       0.1531848   0.031377711
## 4             3       0.1357561   0.007124503
## 5             4       0.1354813   0.005213214
## 6             5       0.1347336   0.005268805
## 7             6       0.1309809   0.003254704
## 8             7       0.1306211   0.005273894
## 9             8       0.1320959   0.005098204
## 10            9       0.1333377   0.006381811
## 11           10       0.1320844   0.005652836
```

Let us now visualize the results and interpret them.

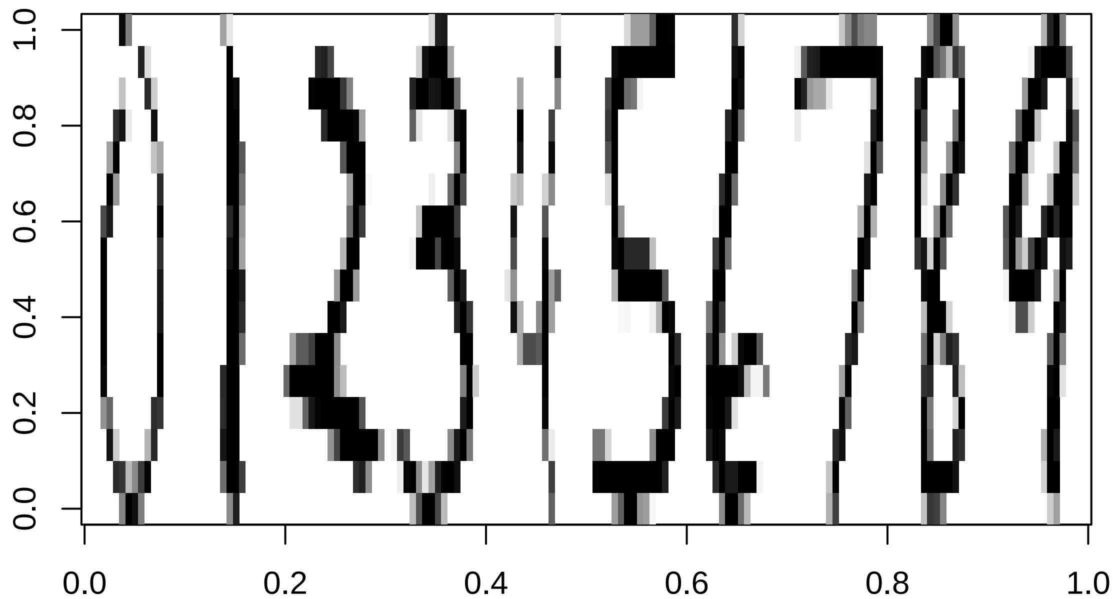


Out of all the models under consideration, the neural network with a single hidden unit performs worst. It has the largest mean average test error and also the largest variation in the average test error for different random starting weights. Somewhat surprisingly, the linear model, i.e. the neural network with no hidden units, performs almost as good as the neural network with two hidden units. While the mean average test errors of these two models are similar, the average test error is much less sensitive to different starting weights in case of the linear model. All neural networks with 3 or more hidden units have a similar performance, both in terms of the mean average test error and the standard deviation of the average test error for different random starting weights. Overall, we conclude that choosing a larger number of hidden units and imposing shrinkage via weight decay appears to be better than having too few hidden units in the first place.

Exercise 2

The data sets `zip.train` and `zip.test` from package **ElemStatLearn** contain information on the gray color values of the pixels on a 16×16 pixel image of hand-written digits. We first visualize for each digit one randomly selected observation.

```
## [1] "digit  0  taken"
## [1] "digit  1  taken"
## [1] "digit  2  taken"
## [1] "digit  3  taken"
## [1] "digit  4  taken"
## [1] "digit  5  taken"
## [1] "digit  6  taken"
## [1] "digit  7  taken"
## [1] "digit  8  taken"
## [1] "digit  9  taken"
```



We now fit a multinomial logistic regression model to the training data and evaluate it on the training and the test data. Before fitting the model, however, we transform the data such that the regressors are scaled on the unit interval.

```
## # weights:  2580 (2313 variable)
## initial  value 16788.147913
## iter  10 value 2894.781800
## iter  20 value 1387.388893
## iter  30 value 805.767631
## iter  40 value 512.133103
## iter  50 value 274.070966
## iter  60 value 196.424106
## iter  70 value 148.210904
## iter  80 value 107.021614
## iter  90 value 72.525058
## iter 100 value 42.177330
## final  value 42.177330
## stopped after 100 iterations
```

We now determine the overall misclassification rate on the training and the test data and the digit-specific misclassification rates on the test data.

```
## [1] "misclassification rate (training data): 0.01%"
```

```
## [1] "misclassification rate (test data): 12.11%"
```

```
## [1] "digit-specific misclassification rates (test data):"
```

```
##         0        1        2        3        4        5        6        7
```

```
##   "3.9%"  "4.55%" "18.69%" "14.46%"    "21%" "16.88%"  "9.41%" "14.29%"
##        8        9
## "22.89%"  "6.78%"
```

The misclassification rate on the training data is exceptionally low, while the one on the test data is fairly high. The digits 8,4 and 2 are particularly difficult to classify, whereas the model does a good job in classifying 0,1, and 9.

The substantial discrepancy in performance between training and test data suggests that overfitting may be an issue. Hence, we add a positive weight decay of 0.05 when fitting the multinomial logistic regression model in order to regularize it.

```
## # weights:  2580 (2313 variable)
## initial  value 16788.147913
## iter  10 value 2909.202379
## iter  20 value 1423.990004
## iter  30 value 894.021900
## iter  40 value 614.653802
## iter  50 value 455.360357
## iter  60 value 417.148011
## iter  70 value 395.150898
## iter  80 value 384.312406
## iter  90 value 378.834838
## iter 100 value 376.137836
## final  value 376.137836
## stopped after 100 iterations
```

```
## [1] "misclassification rate (training data): 0.3%"
```

```
## [1] "misclassification rate (test data): 9.32%"
```

```
## [1] "digit-specific misclassification rates (test data):"
```

```
##        0        1        2        3        4        5        6        7
##   "3.9%"  "4.55%" "15.66%" "10.84%"  "13.5%" "13.75%"  "7.65%"  "10.2%"
##        8        9
## "15.06%"  "5.65%"
```

Adding weight decay slightly increases the misclassification rate on the training data, but reduces the misclassification rate on the test data. The improved classification performance is particularly pronounced for the “difficult’ ’ digits (8 and 4). Overall, adding a Ridge penalty to the loss function, i.e. adding the weight decay, improves the out-of-sample performance of our model by mitigating the overfitting problem.

Exercise 3

We continue using the data sets `zip.train` and `zip.test` from package **ElemStatLearn**. However, we now only use a subset of size 320 from *zip.train*, with an equal number of observations for each digit to fit a multinomial logistic regression model and a neural network. We use the remaining observations from `zip.train` and the test data to evaluate the fitted models.

Given the small sample size of the training data, overfitting is most likely an issue. We therefore visualize the performance on the test data in dependence of the training epochs when fitting the models.

```
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## final  value 48.364930
## stopped after 10 iterations
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## iter  20 value 0.871059
## final  value 0.871059
## stopped after 20 iterations
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## iter  20 value 0.871059
## iter  30 value 0.071842
## final  value 0.071842
## stopped after 30 iterations
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## iter  20 value 0.871059
## iter  30 value 0.071842
## iter  40 value 0.024620
## iter  50 value 0.012972
## final  value 0.012972
## stopped after 50 iterations
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## iter  20 value 0.871059
## iter  30 value 0.071842
## iter  40 value 0.024620
## iter  50 value 0.012972
## iter  60 value 0.006339
## iter  70 value 0.003518
## iter  80 value 0.002358
## iter  90 value 0.001610
## iter 100 value 0.000943
## final  value 0.000943
## stopped after 100 iterations
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## iter  20 value 0.871059
```

```
## iter  30 value 0.071842
## iter  40 value 0.024620
## iter  50 value 0.012972
## iter  60 value 0.006339
## iter  70 value 0.003518
## iter  80 value 0.002358
## iter  90 value 0.001610
## iter 100 value 0.000943
## iter 110 value 0.000645
## iter 120 value 0.000491
## iter 130 value 0.000251
## iter 140 value 0.000245
## iter 150 value 0.000148
## final  value 0.000148
## stopped after 150 iterations
## # weights:  2580 (2313 variable)
## initial  value 736.827230
## iter  10 value 48.364930
## iter  20 value 0.871059
## iter  30 value 0.071842
## iter  40 value 0.024620
## iter  50 value 0.012972
## iter  60 value 0.006339
## iter  70 value 0.003518
## iter  80 value 0.002358
## iter  90 value 0.001610
## iter 100 value 0.000943
## iter 110 value 0.000645
## iter 120 value 0.000491
## iter 130 value 0.000251
## iter 140 value 0.000245
## iter 150 value 0.000148
## final  value 0.000097
## converged
```

```
## # weights:  3905
## initial  value 1663.464935
## iter  10 value 79.681992
## final  value 79.681992
## stopped after 10 iterations
## # weights:  3905
## initial  value 1672.904167
## iter  10 value 72.661942
## iter  20 value 2.169041
## final  value 2.169041
## stopped after 20 iterations
## # weights:  3905
## initial  value 1718.087019
## iter  10 value 26.083447
## iter  20 value 0.310144
## iter  30 value 0.027409
## final  value 0.027409
## stopped after 30 iterations
## # weights:  3905
```

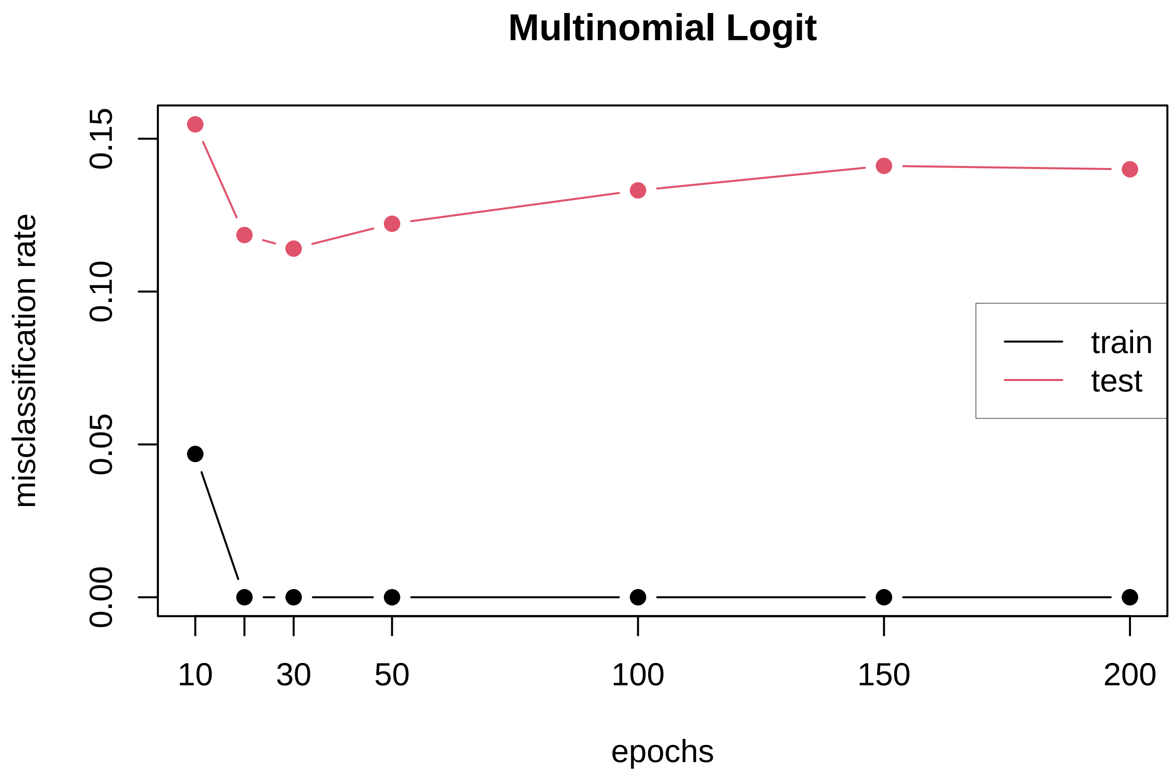
```
## initial  value 1414.276942
## iter  10 value 49.144805
## iter  20 value 0.711485
## iter  30 value 0.040968
## iter  40 value 0.012149
## iter  50 value 0.005050
## final  value 0.005050
## stopped after 50 iterations
## # weights:  3905
## initial  value 1423.970760
## iter  10 value 51.484734
## iter  20 value 1.462150
## iter  30 value 0.075633
## iter  40 value 0.017703
## iter  50 value 0.007656
## iter  60 value 0.003753
## iter  70 value 0.001567
## iter  80 value 0.001186
## iter  90 value 0.000469
## iter 100 value 0.000376
## final  value 0.000376
## stopped after 100 iterations
## # weights:  3905
## initial  value 1716.030320
## iter  10 value 53.207437
## iter  20 value 0.907040
## iter  30 value 0.056523
## iter  40 value 0.014348
## iter  50 value 0.005803
## iter  60 value 0.003249
## iter  70 value 0.001491
## iter  80 value 0.001056
## iter  90 value 0.000716
## iter 100 value 0.000387
## iter 110 value 0.000318
## iter 120 value 0.000176
## iter 130 value 0.000171
## final  value 0.000079
## converged
## # weights:  3905
## initial  value 1945.337703
## iter  10 value 93.956697
## iter  20 value 0.499032
## iter  30 value 0.065199
## iter  40 value 0.019139
## iter  50 value 0.007662
## iter  60 value 0.003780
## iter  70 value 0.002467
## iter  80 value 0.001238
## iter  90 value 0.000932
## iter 100 value 0.000293
## iter 110 value 0.000255
## iter 120 value 0.000223
## final  value 0.000092
```

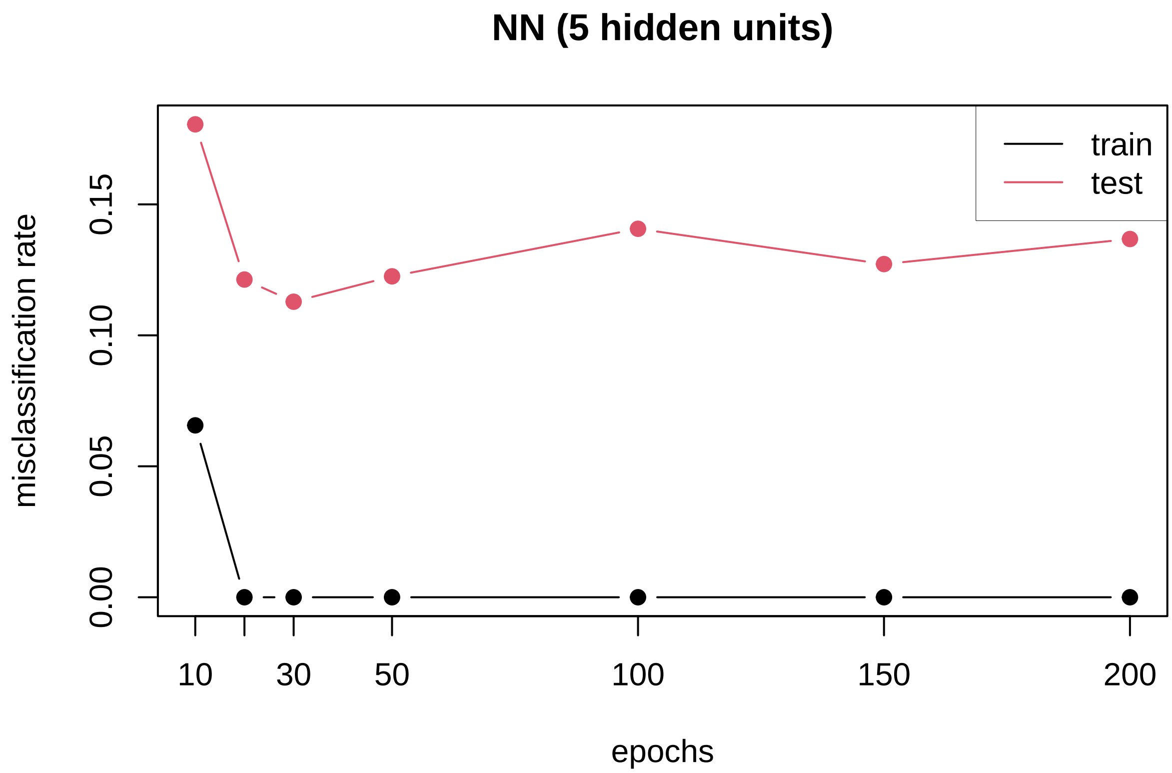
```
## converged
## # weights:  5240
## initial  value 1733.045132
## iter  10 value 34.775126
## final  value 34.775126
## stopped after 10 iterations
## # weights:  5240
## initial  value 1775.725557
## iter  10 value 48.130639
## iter  20 value 0.940412
## final  value 0.940412
## stopped after 20 iterations
## # weights:  5240
## initial  value 2019.009483
## iter  10 value 65.782554
## iter  20 value 0.447219
## iter  30 value 0.035726
## final  value 0.035726
## stopped after 30 iterations
## # weights:  5240
## initial  value 1830.764123
## iter  10 value 109.463346
## iter  20 value 0.604526
## iter  30 value 0.034259
## iter  40 value 0.007428
## iter  50 value 0.003200
## final  value 0.003200
## stopped after 50 iterations
## # weights:  5240
## initial  value 1862.966329
## iter  10 value 112.738462
## iter  20 value 1.364118
## iter  30 value 0.054795
## iter  40 value 0.010239
## iter  50 value 0.003593
## iter  60 value 0.001317
## iter  70 value 0.000752
## iter  80 value 0.000446
## iter  90 value 0.000247
## iter 100 value 0.000179
## final  value 0.000179
## stopped after 100 iterations
## # weights:  5240
## initial  value 2257.881719
## iter  10 value 138.424472
## iter  20 value 2.937467
## iter  30 value 0.086749
## iter  40 value 0.016862
## iter  50 value 0.004691
## iter  60 value 0.002354
## iter  70 value 0.001360
## iter  80 value 0.000739
## iter  90 value 0.000341
```

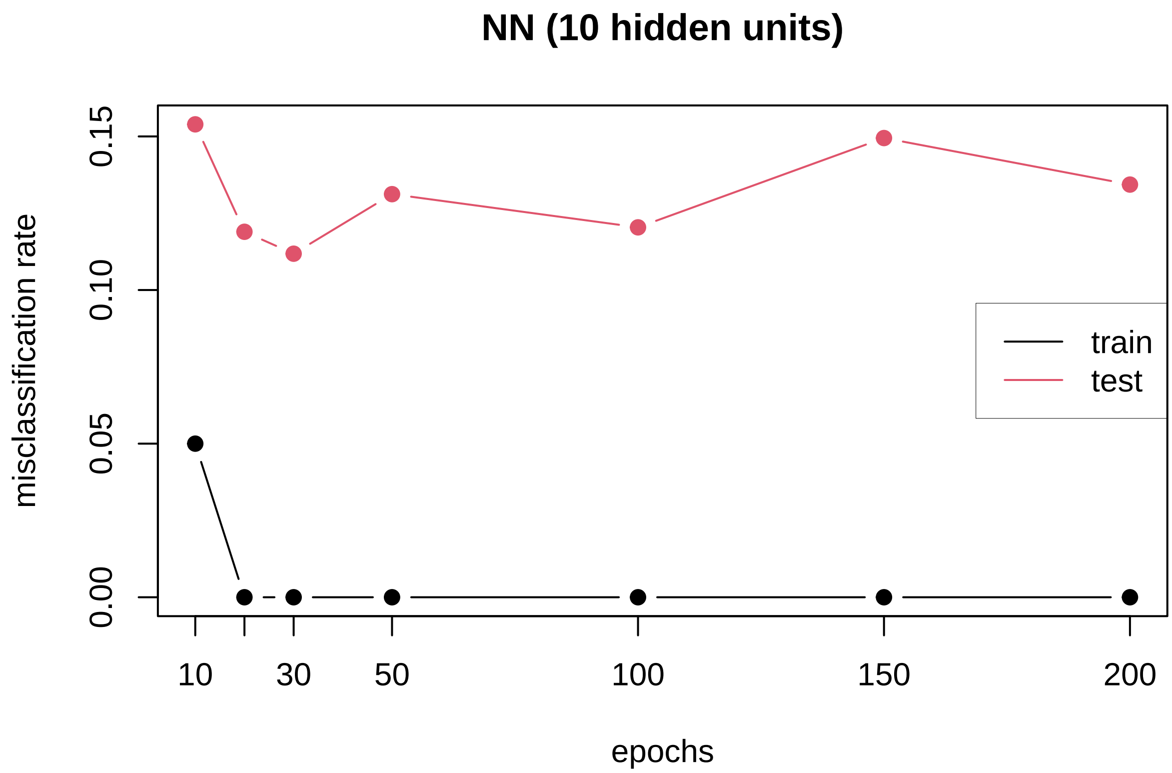
```
## iter 100 value 0.000231
## final  value 0.000094
## converged
## # weights:  5240
## initial  value 1815.038186
## iter  10 value 71.281739
## iter  20 value 0.655870
## iter  30 value 0.048885
## iter  40 value 0.011945
## iter  50 value 0.004802
## iter  60 value 0.002787
## iter  70 value 0.001407
## iter  80 value 0.000837
## iter  90 value 0.000416
## iter 100 value 0.000232
## iter 110 value 0.000164
## iter 120 value 0.000146
## final  value 0.000099
## converged
```

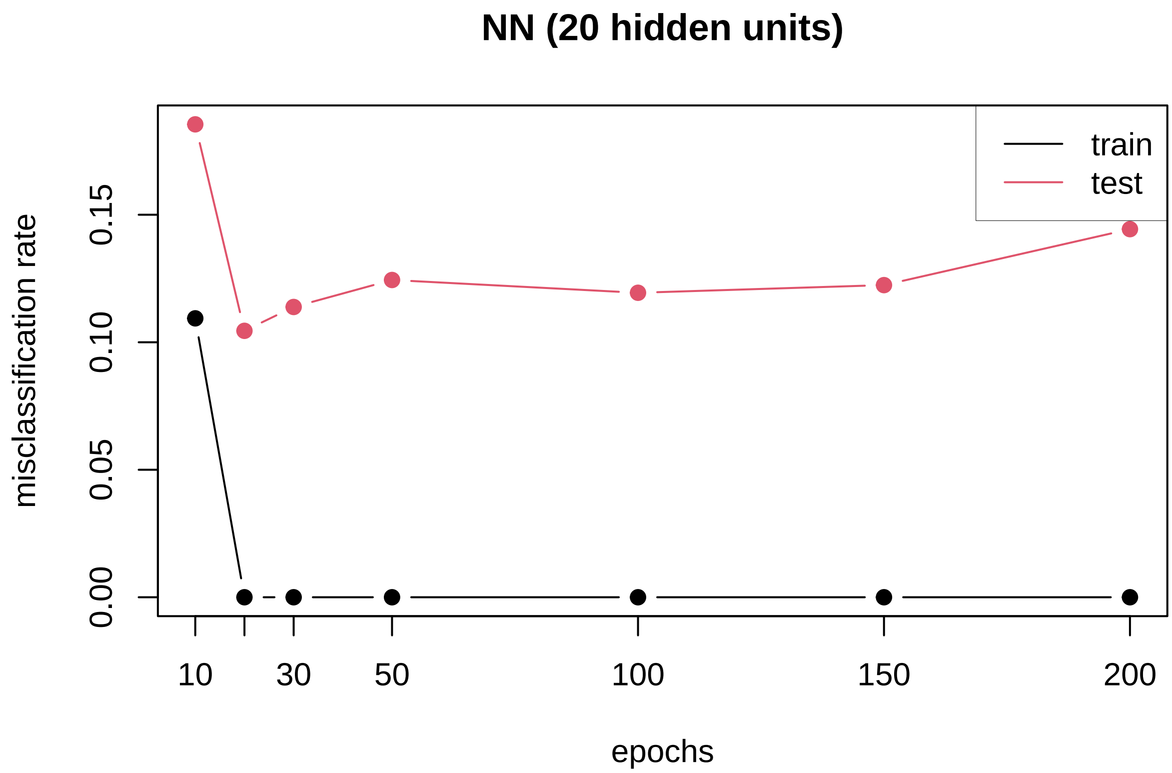
```
## # weights:  7910
## initial  value 1881.948733
## iter  10 value 109.088936
## final  value 109.088936
## stopped after 10 iterations
## # weights:  7910
## initial  value 1452.629520
## iter  10 value 18.532800
## iter  20 value 0.301964
## final  value 0.301964
## stopped after 20 iterations
## # weights:  7910
## initial  value 1707.344006
## iter  10 value 55.575636
## iter  20 value 0.553530
## iter  30 value 0.039971
## final  value 0.039971
## stopped after 30 iterations
## # weights:  7910
## initial  value 1663.993040
## iter  10 value 61.140362
## iter  20 value 1.455502
## iter  30 value 0.049836
## iter  40 value 0.008999
## iter  50 value 0.003133
## final  value 0.003133
## stopped after 50 iterations
## # weights:  7910
## initial  value 1577.776309
## iter  10 value 19.437617
## iter  20 value 0.447892
## iter  30 value 0.023991
## iter  40 value 0.005424
## iter  50 value 0.002308
```

```
## iter  60 value 0.001038
## iter  70 value 0.000399
## iter  80 value 0.000315
## iter  90 value 0.000161
## iter 100 value 0.000130
## final  value 0.000130
## stopped after 100 iterations
## # weights:  7910
## initial  value 1367.205805
## iter  10 value 79.214546
## iter  20 value 0.815774
## iter  30 value 0.030266
## iter  40 value 0.007252
## iter  50 value 0.003066
## iter  60 value 0.001554
## iter  70 value 0.000748
## iter  80 value 0.000539
## iter  90 value 0.000214
## iter 100 value 0.000168
## final  value 0.000092
## converged
## # weights:  7910
## initial  value 1653.554576
## iter  10 value 85.165965
## iter  20 value 3.621547
## iter  30 value 0.089329
## iter  40 value 0.005340
## iter  50 value 0.001577
## iter  60 value 0.000309
## iter  70 value 0.000187
## final  value 0.000096
## converged
```


Multinomial Logit
misclassification rate
0.00
0.05
0.10
0.15
10
30
50
100
150
200
epochs
train
test


NN (5 hidden units)
train
test
misclassification rate
0.00
0.05
0.10
0.15
10
30
50
100
150
200
epochs


NN (10 hidden units)
misclassification rate
0.00
0.05
0.10
0.15
10
30
50
100
150
200
epochs
train
test

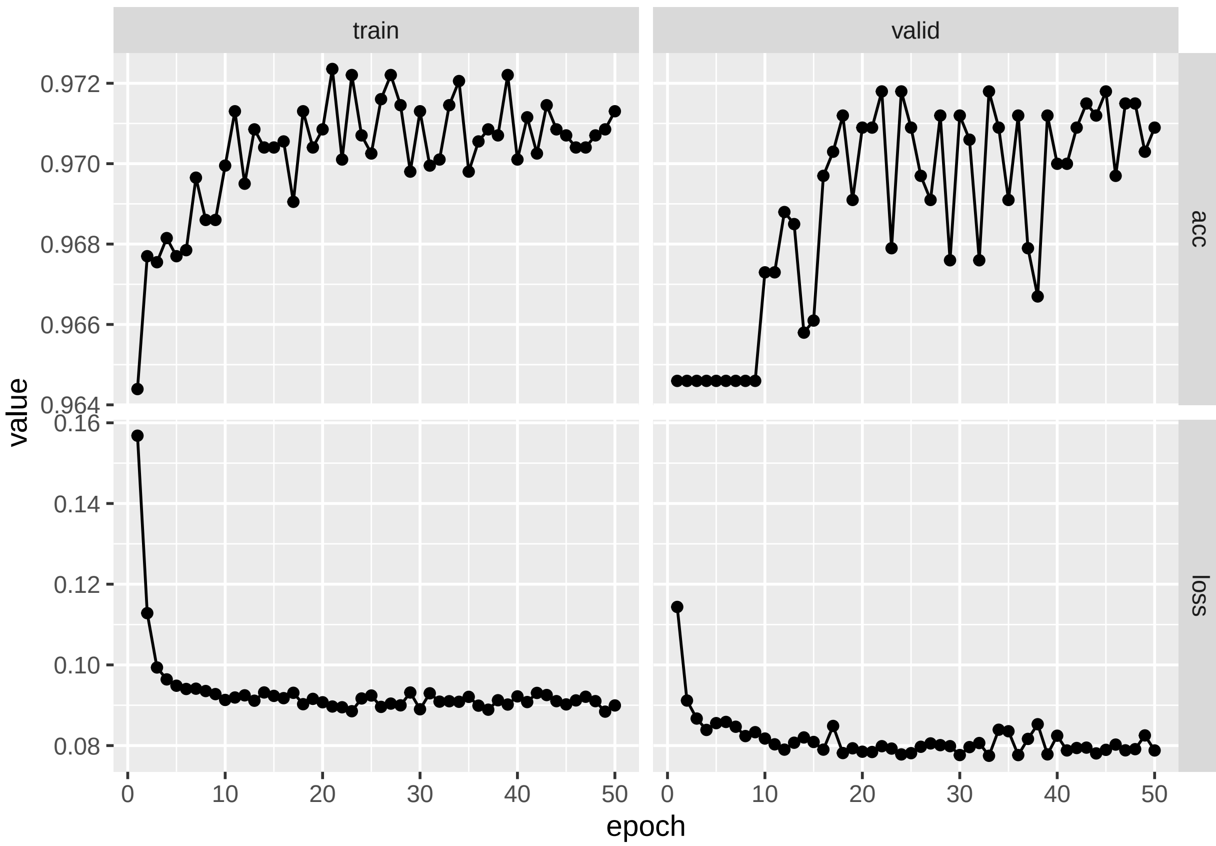


The plots are in line with our assumption that overfitting is an issue in this exercise. For all models (multinomial logit, neural networks with 5, 10 and 20 hidden units) the misclassification rate on the test data increases as the number of training epochs exceeds 30. Hence, in the absence of a more explicit form of regularization (e.g. a positive weight decay) stopping the optimization routine early can be helpful to improve out-of-sample performance.

Exercise 4

In the following we will estimate a predictive model for the `Default` data from the **ISLR2** pacakge. We fit a neural network using a single hidden layer with 10 units and dropout regularization.

```
##   default student   balance    income
## 1      No      No  729.5265 44361.625
## 2      No     Yes  817.1804 12106.135
## 3      No      No 1073.5492 31767.139
## 4      No      No  529.2506 35704.494
## 5      No      No  785.6559 38463.496
## 6      No     Yes  919.5885  7491.559
```



The linear logistic regression model performs very well on the test data and has a classification accuracy of 97.18. Our neural network also performs quite well and has a slightly lower accuracy of 97.09. Looking at the plots above, we can see that the value of the loss function decreases as the number of training epochs increases - for both the training and the test data. Given that the loss function evaluated at the test data does not increase as the number of epochs grows larger, we find no evidence for overfitting. The classification performance slightly improves as the number of training epochs increases. However, it does not improve monotonically and the marginal gains are rather negligible.

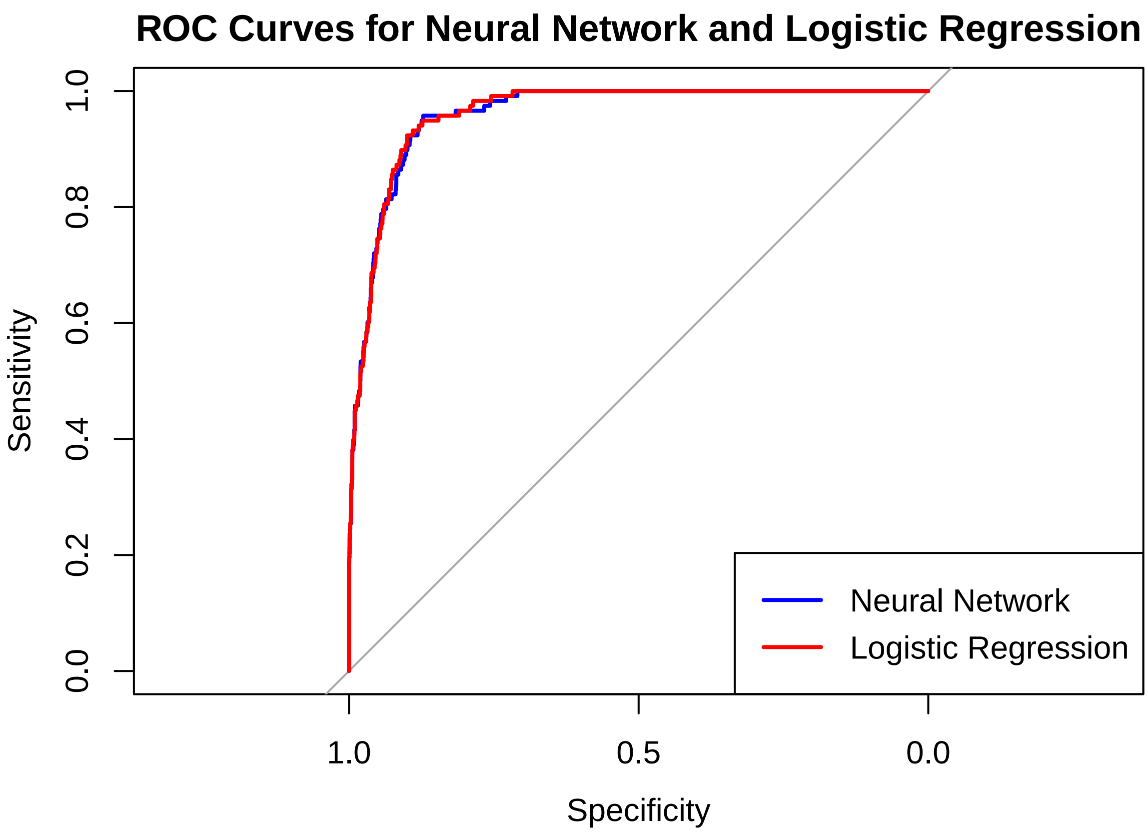
We now compare the classification performance of the two models more closely.

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

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

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

```
##
##     cov, smooth, var
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases
```




```
## AUC for Neural Network: 0.9611066
## AUC for Logistic Regression: 0.9622321
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##          0 3212   94
##          1    3   24
##
##                Accuracy : 0.9709
##                  95% CI : (0.9646, 0.9763)
##     No Information Rate : 0.9646
##     P-Value [Acc > NIR] : 0.02474
##
##                   Kappa : 0.3221
##
```

```
##  Mcnemar's Test P-Value : < 2e-16
##
##             Sensitivity : 0.9991
##             Specificity : 0.2034
##          Pos Pred Value : 0.9716
##          Neg Pred Value : 0.8889
##              Prevalence : 0.9646
##          Detection Rate : 0.9637
##    Detection Prevalence : 0.9919
##       Balanced Accuracy : 0.6012
##
##        'Positive' Class : 0
##

## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##          0 3202   81
##          1   13   37
##
##                Accuracy : 0.9718
##                  95% CI : (0.9656, 0.9772)
##     No Information Rate : 0.9646
##     P-Value [Acc > NIR] : 0.01177
##
##                   Kappa : 0.4284
##
##  Mcnemar's Test P-Value : 4.829e-12
##
##             Sensitivity : 0.9960
##             Specificity : 0.3136
##          Pos Pred Value : 0.9753
##          Neg Pred Value : 0.7400
##              Prevalence : 0.9646
##          Detection Rate : 0.9607
##    Detection Prevalence : 0.9850
##       Balanced Accuracy : 0.6548
##
##        'Positive' Class : 0
##
```

Exercise 5

Now we perform document classification on the *IMDb* data set, which is available as part of the **torchdatasets** package. We limit the dictionary size to the 10,000 most frequently-used words and tokens. Again, we use James et al. (2021, Chapter 10). We begin by loading the data and creating a imdb_tain and imdb_test object. Each element of imdb_train is a vector of numbers between 1 and 10000 (the document), referring to the words found in the dictionary. Next we write a function to one-hot encode each document in a list of documents, and return a binary matrix in sparse-matrix format. To construct the sparse matrix, one supplies just the entries that are nonzero. In the last line we call the function sparseMatrix() and supply the row indices corresponding to each document and the column indices corresponding to the words in each document, since we omit the values they are taken to be all ones. Words that appear more than once in any given document still get recorded as a one.

Consider the effects of varying the dictionary size. Try the values 500, 1000, 3000, 5000, and 10,000, and compare the results.