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.

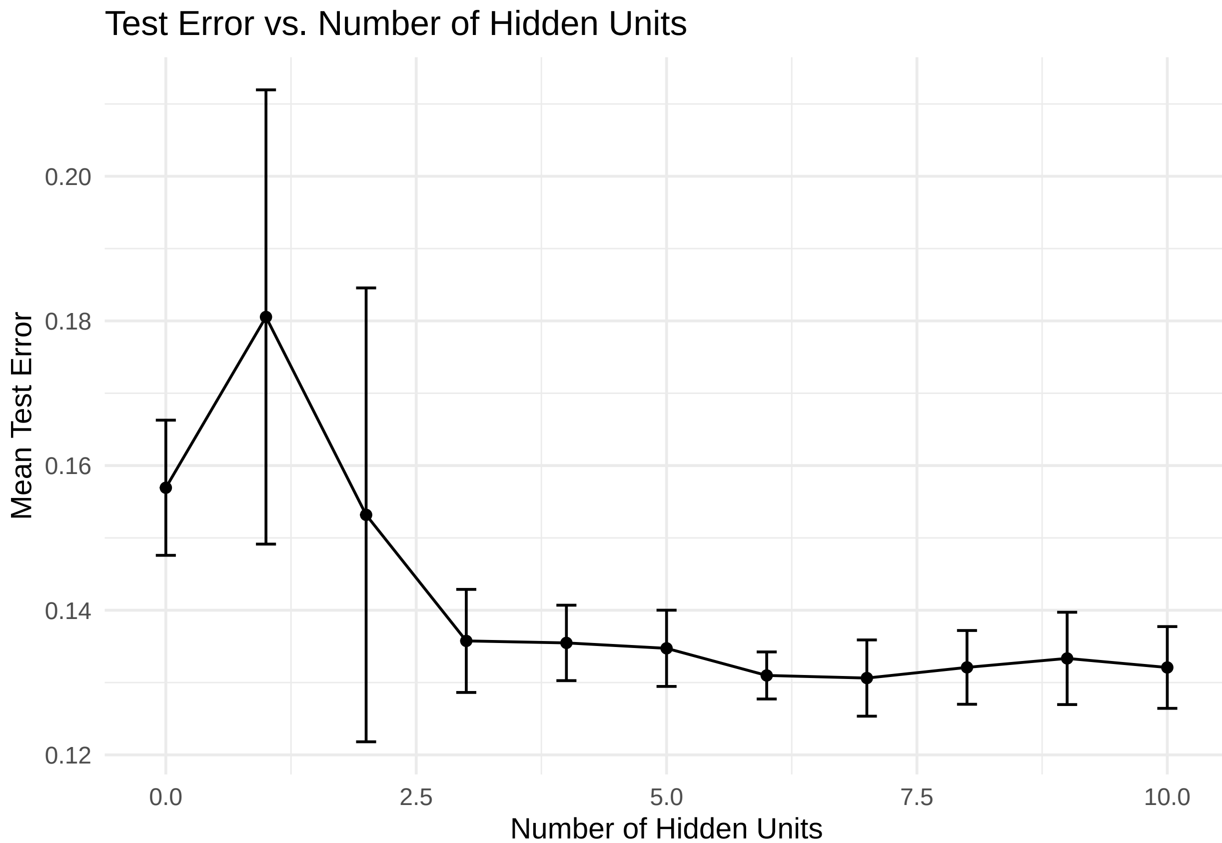
We then fit neural networks with weight decay of 0.0005 and vary the number of hidden units from 0 to 10. We record the average test error

$$\mathbb{E}_{\text{Test}}(Y - \hat{f}(X_1, X_2))^2$$

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
```

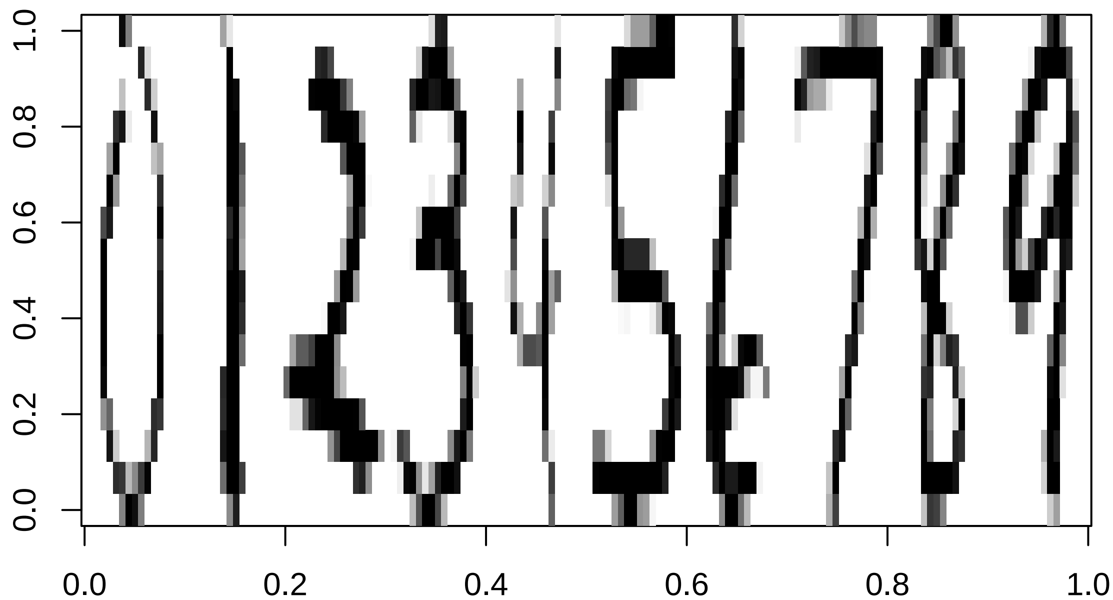
Let us now visualize the results and interpret them.



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.



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.

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.

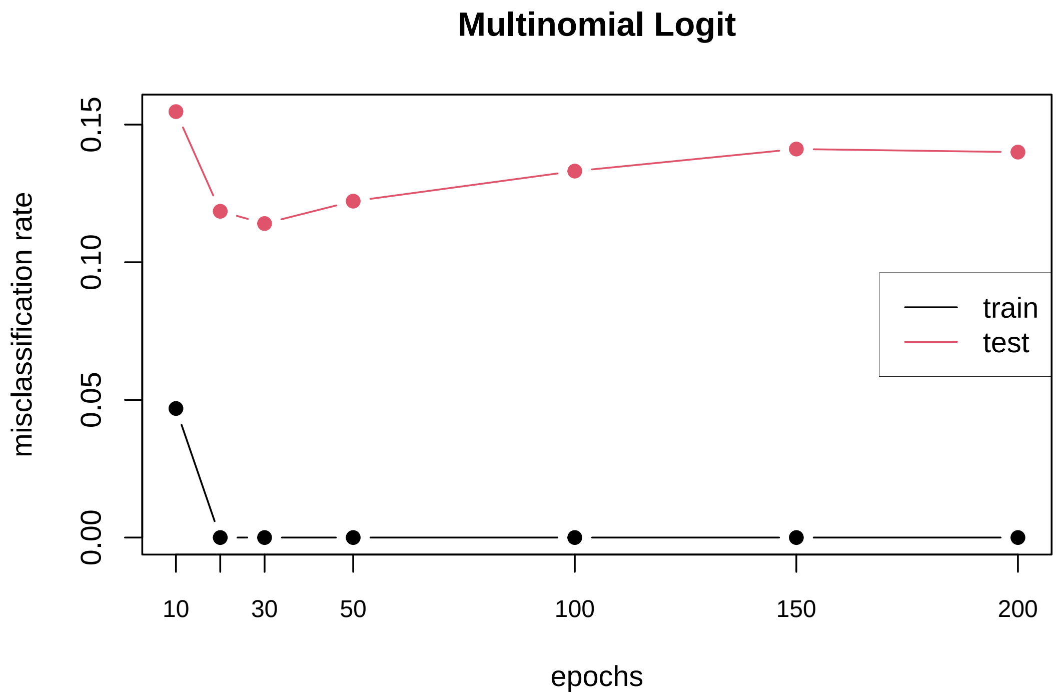
```
## [1] "misclassification rate (training data): 0.3%"

## [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%"
```

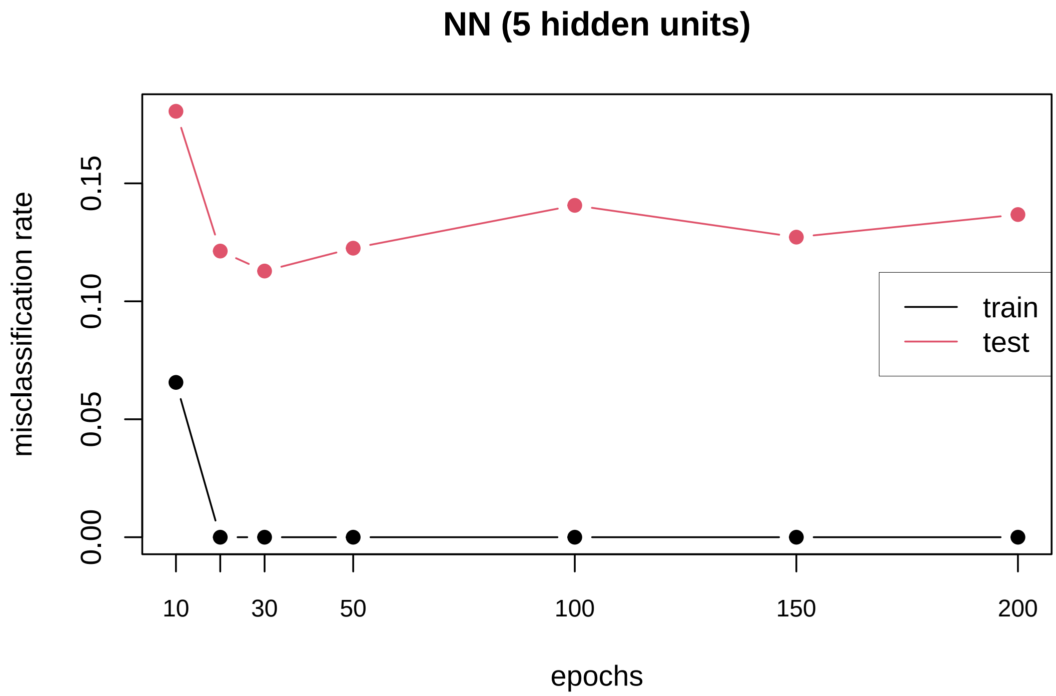
Adding weight decay slightly increases the misclassification rate on the training data, but reduces the misclassification rate on the test data. The improved classification performance is particularly pronounced for the "difficult" digits (8 and 4). Overall, adding a Ridge penalty to the loss function,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

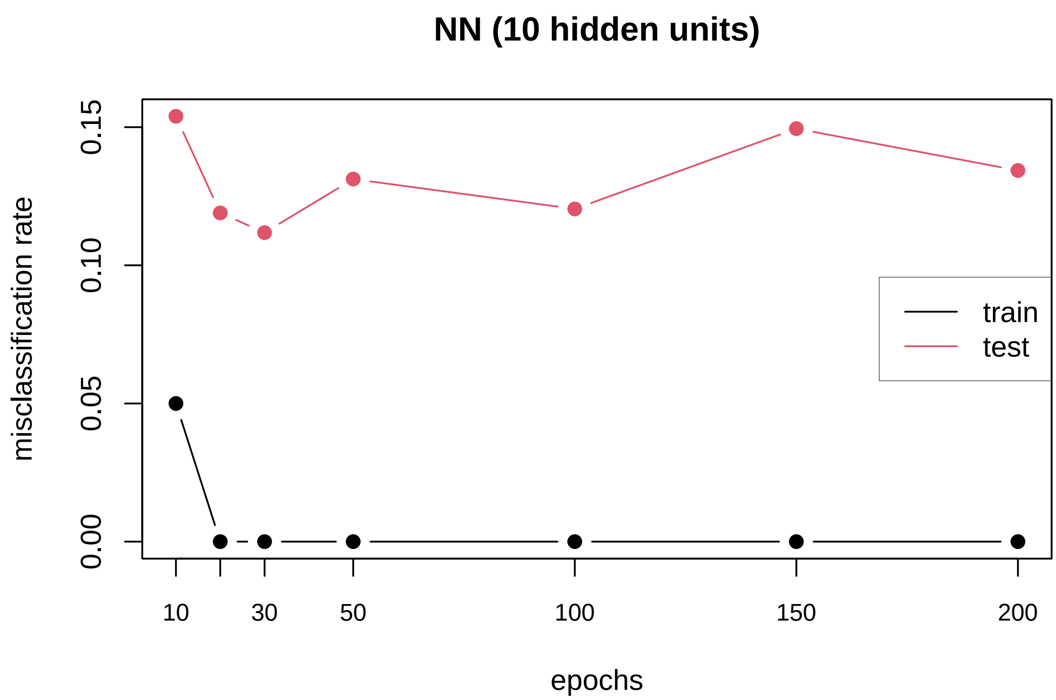
Exercise 3

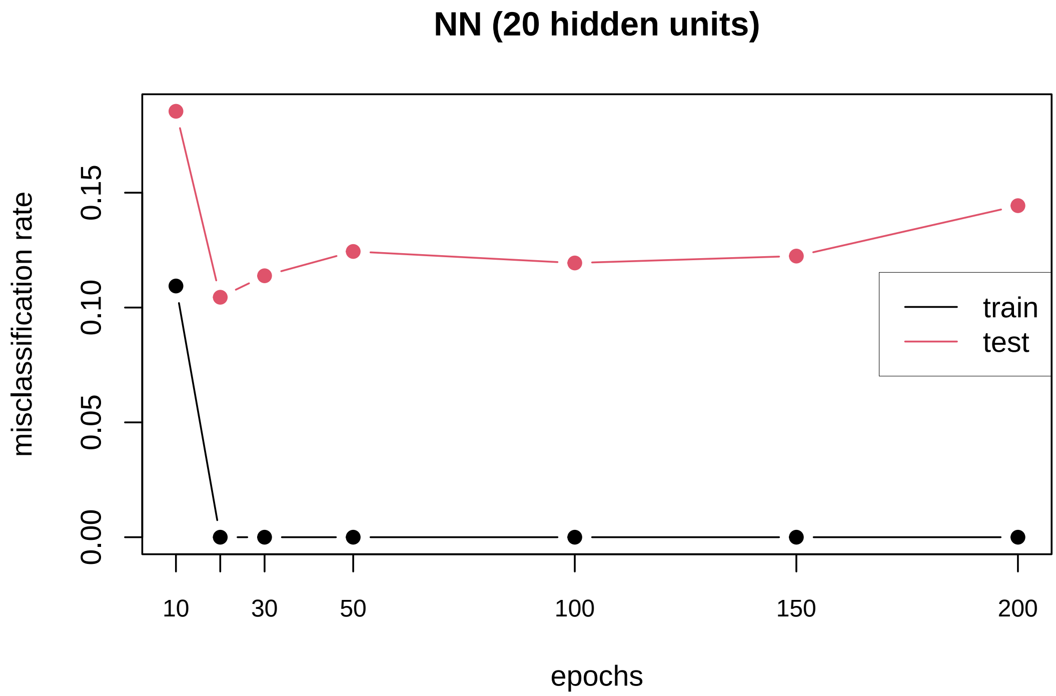
We continue using the data sets `zip.train` and `zip.test` from package **ElemStatLearn**. However, we now only use a subset of size 320 from `zip.train`, with an equal number of observations for each digit to fit a multinomial logistic regression model and a neural network. We use the remaining observations 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 (# epochs $\in \{10, 20, 30, 50, 100, 150, 200\}$) when fitting the models.




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

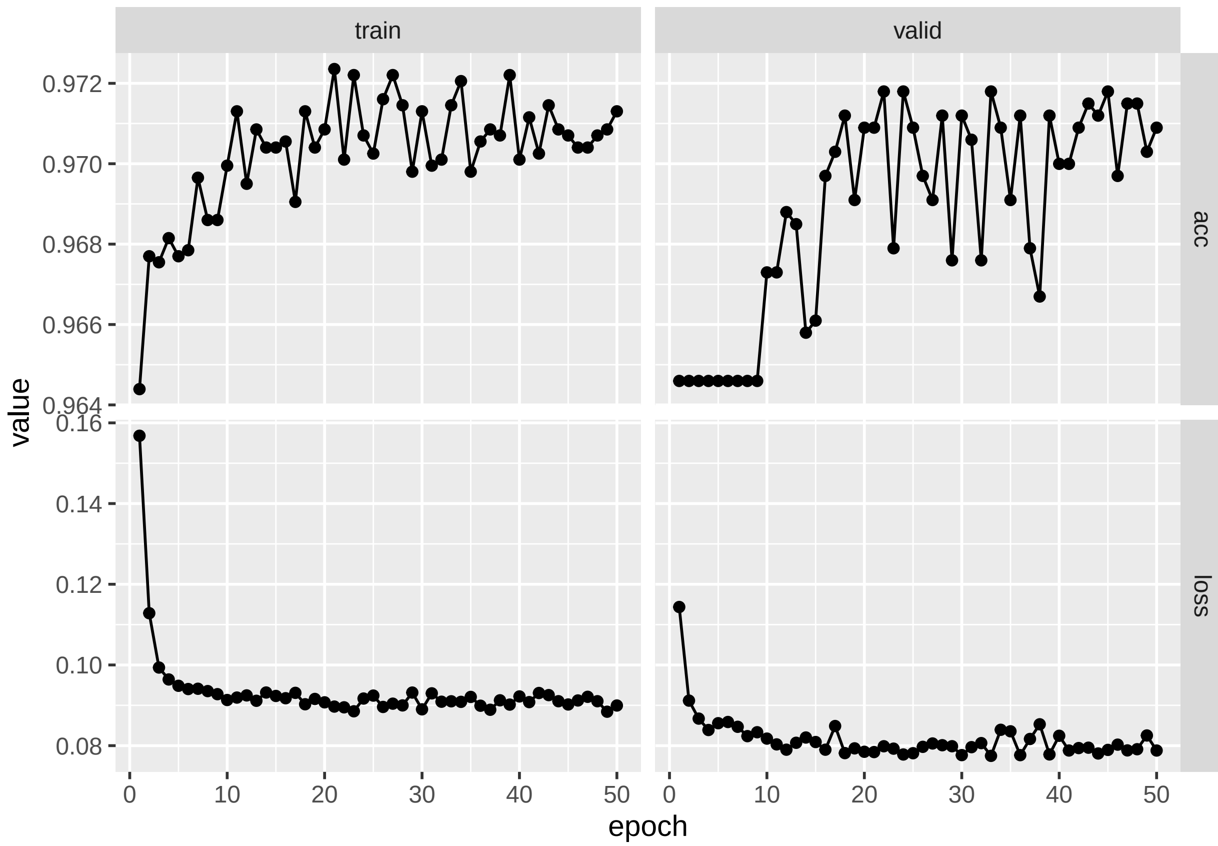

NN (10 hidden units)
misclassification rate
0.00
0.05
0.10
0.15
10
30
50
100
150
200
epochs
train
test



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

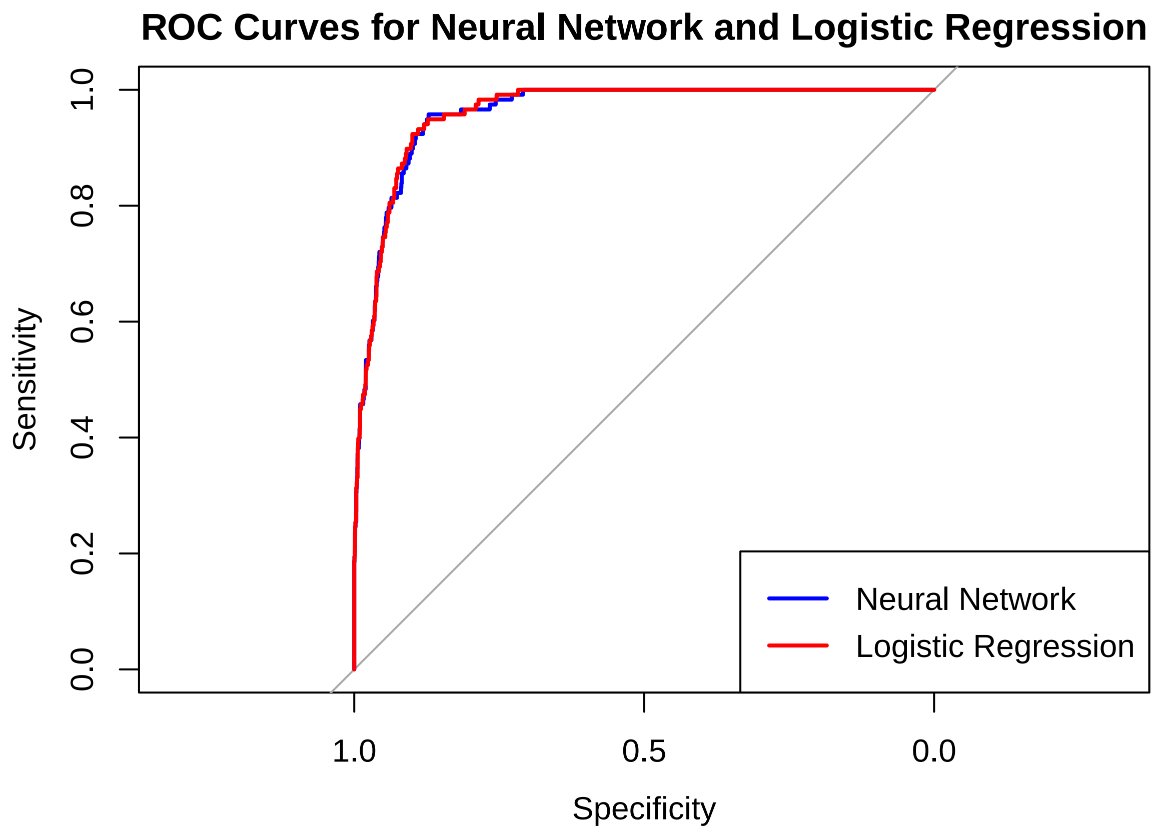
In the following we will estimate a predictive model for the `Default` data from the **ISLR2** package. We fit a neural network using a single hidden layer with 10 units and dropout regularization.



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 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, by looking at their ROC curve and confusion matrix. In the ROC plot we observe that the curves for the linear logistic regression model and the neural network follow each other closely. The confusion matrices, however, highlight some subtle differences between the two models. The logistic regression model predicts almost twice as many defaults (50 in total, 13 of them incorrectly) as the neural network (27 in total, 3 of them incorrectly).

```
## 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

## [1] "Neural Network:"

## 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
##
```

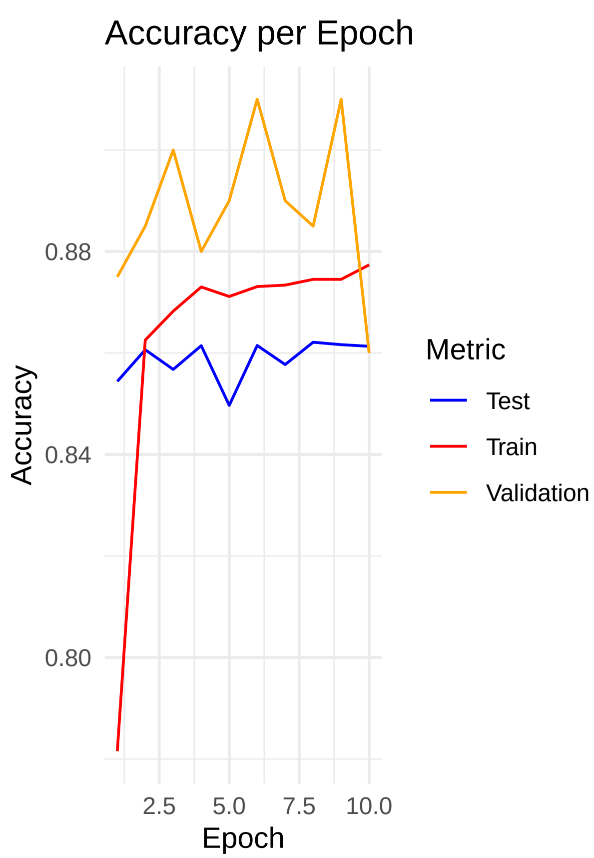
```
## [1] "Logistic Regression:"
```

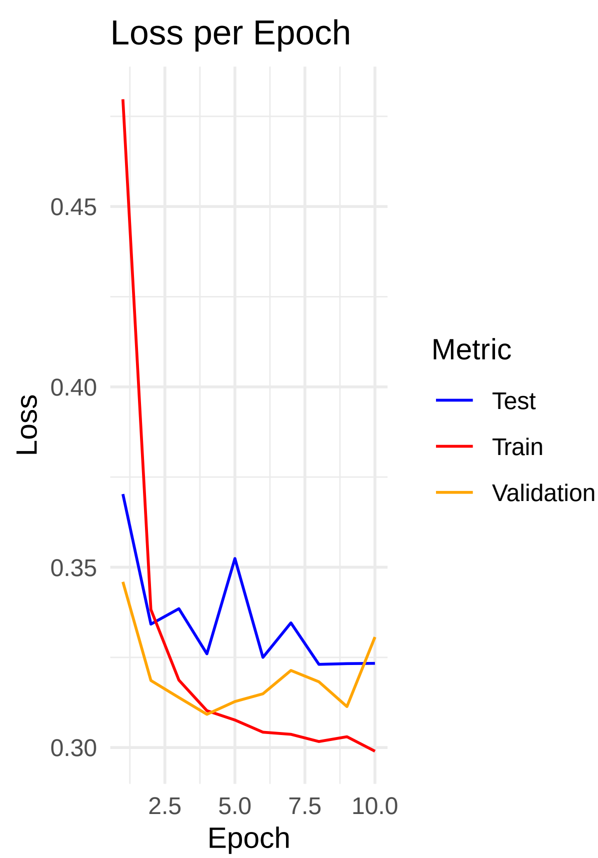
```
## Confusion Matrix and Statistics
##
##           Reference
## Prediction    0    1
##          0 3202   81
##          1   13   37
##
##                Accuracy : 0.9718
##                  95% CI : (0.9656, 0.9772)
##     No Information Rate : 0.9646
##     P-Value [Acc > NIR] : 0.01177
##
##                   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

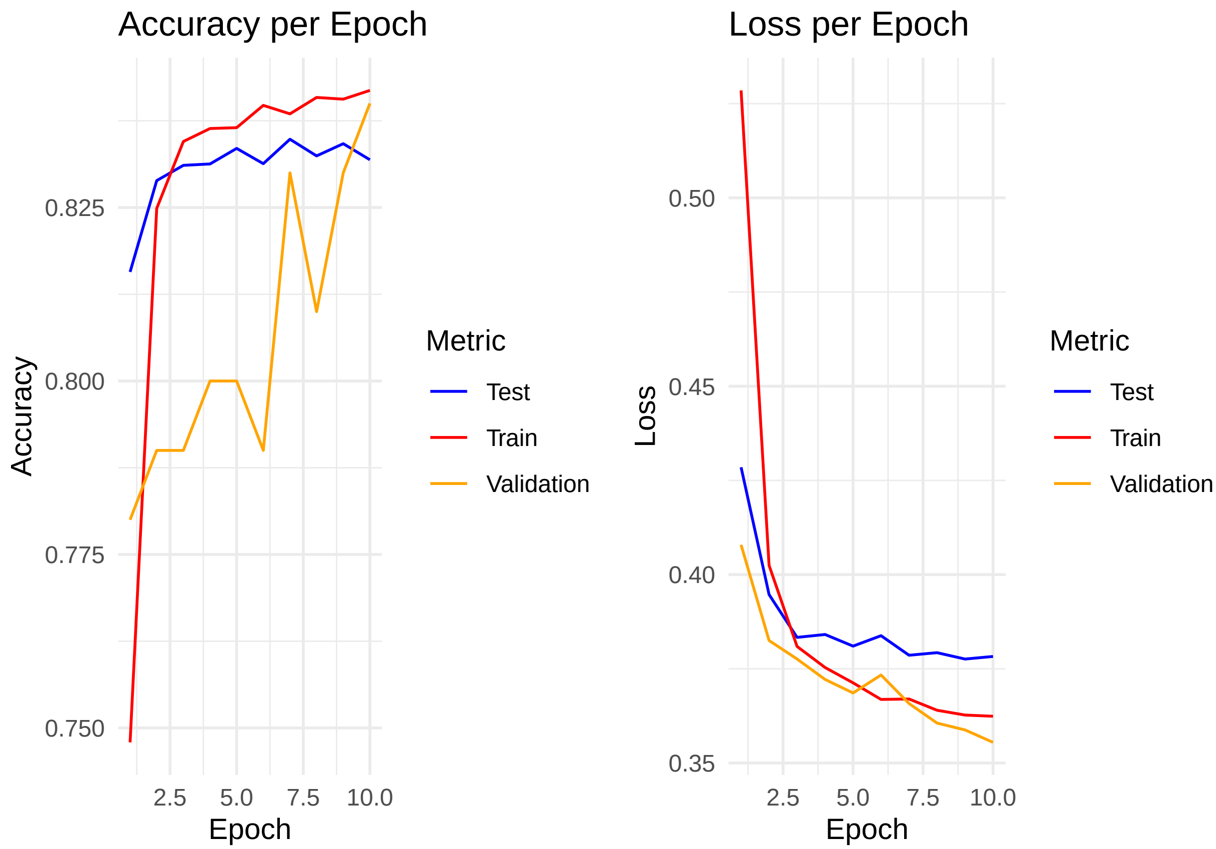
Now we perform document classification on the `IMDb` data set, which is available as part of the **torchdatasets** package. We limit the dictionary size to the 10,000 most frequently-used words and tokens. Again, we use James et al. (2021, Chapter 10 torch version). We begin by loading the data and creating 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. Next we fit a fully-connected neural network with two hidden layers, each with 16 units and ReLU activation.

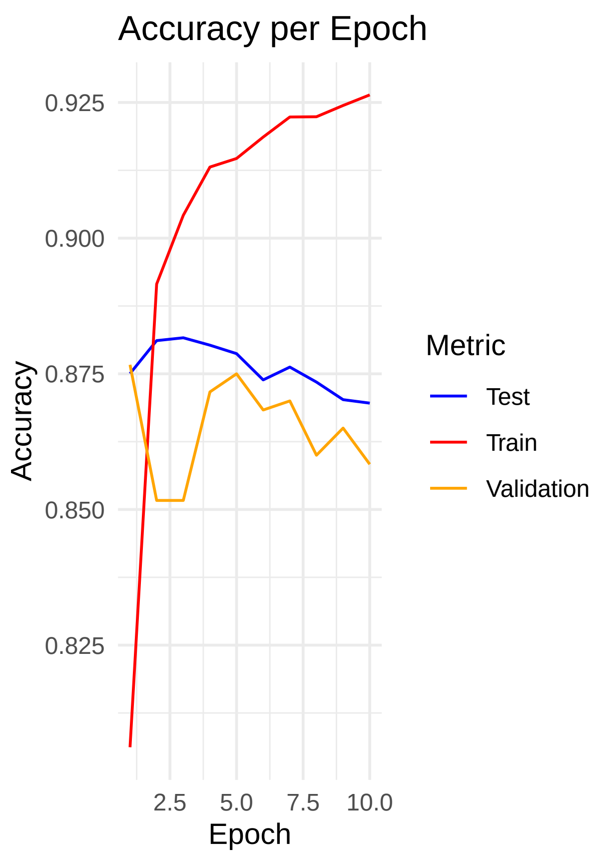
After fitting the fully-connected neural network we can now look at the results with the dictionary size 1000. We look at how the accuracy and the loss of our train, test and validation set evolve over 10 epochs. The accuracy graph displays that for the dictionary size of 1000 the accuracy is highest for the validation set (above 0.88), followed by the train set and lowest for the test set. Also for the train set the accuracy increased sharply after the first 2 epochs. For test and train it starts higher up but has higher variability. Considering the loss, we see a similar development for our train set: For the first 2 epochs the loss is rather high and then drops down and remains at more stable level. The loss for the test and validation sets starts at a lower point again, with the validation loss being below the test loss.

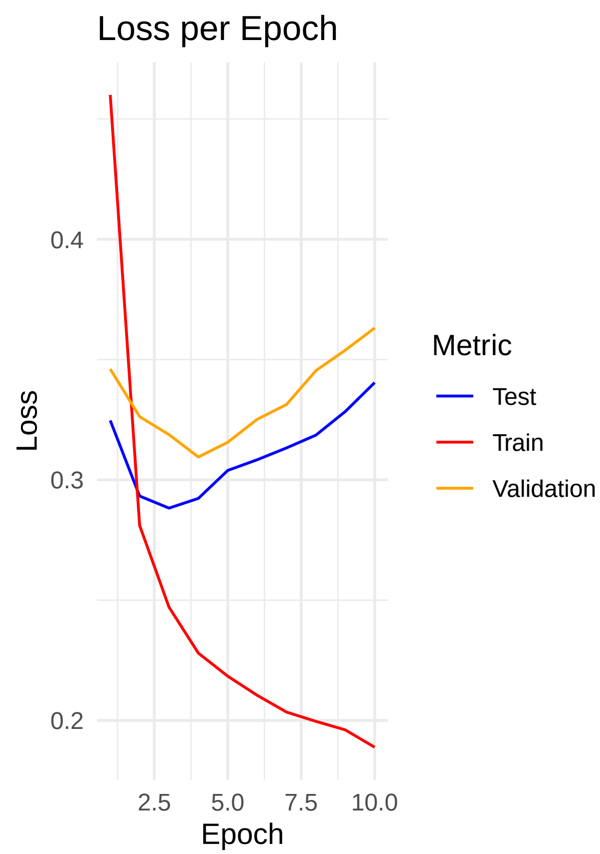


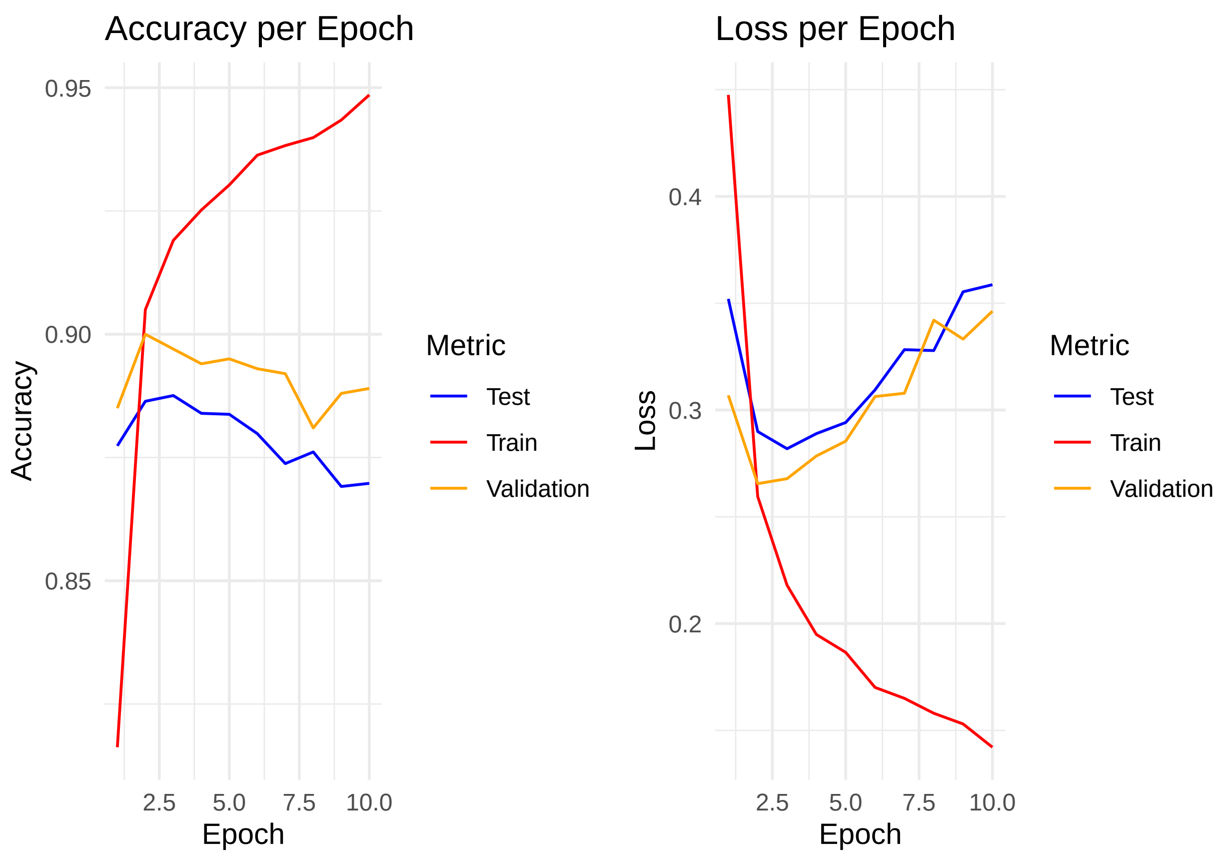


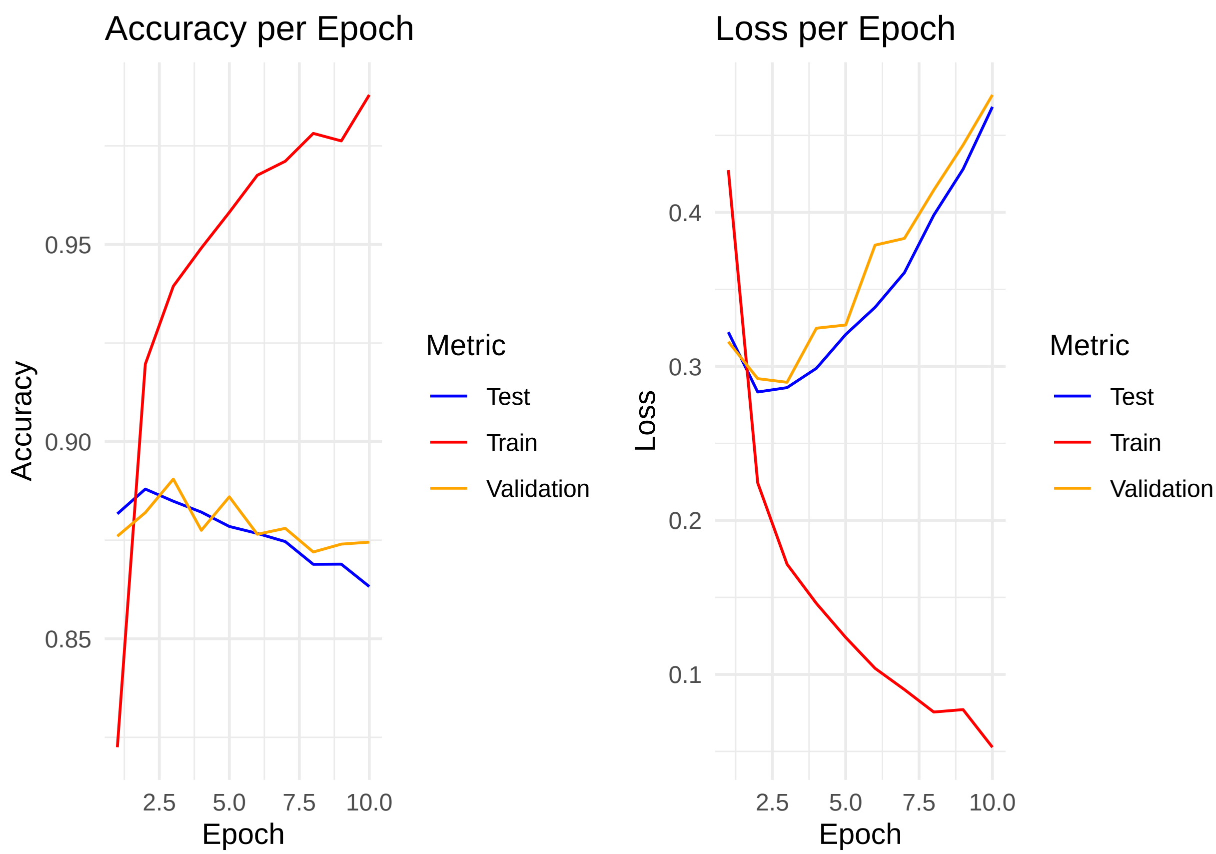
We then vary the dictionary size and try out values 500, 1000, 3000, 5000, 10,000 and consider the effects of this varying dictionary size. We observe that the larger the dictionary size the higher the accuracy (above 0.95 for dictionary size 10,000) and the lower the loss for the training set. Moreover, the higher the accuracy of the training set, the (slightly) higher the accuracy of the validation and test sets. In addition, from the loss plots we can observe that the higher the dictionary size, the more the loss varies between training, test and validation set. Furthermore, the loss for the test set increases strongly with more epochs, while the loss for the training data set decreases (with more epochs).




Accuracy per Epoch
0.925
0.900
0.875
0.850
0.825
Accuracy
2.5
5.0
7.5
10.0
Epoch
Metric
Test
Train
Validation


Loss per Epoch
0.4
0.3
0.2
Loss
2.5
5.0
7.5
10.0
Epoch
Metric
Test
Train
Validation


Accuracy per Epoch
0.95
0.90
0.85
Accuracy
2.5
5.0
7.5
10.0
Epoch
Metric
Test
Train
Validation
Loss per Epoch
0.4
0.3
0.2
Loss
2.5
5.0
7.5
10.0
Epoch
Metric
Test
Train
Validation



Accuracy per Epoch
Accuracy
0.95
0.90
0.85
2.5
5.0
7.5
10.0
Epoch
Metric
Test
Train
Validation
Loss per Epoch
Loss
0.4
0.3
0.2
0.1
2.5
5.0
7.5
10.0
Epoch
Metric
Test
Train
Validation