MLP Coursework 1

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Abstract

In this report we study the problem of overfitting, which is the training regime where performance increases on the training set but decrease on validation data. **[Question 1 - Summarise why overfitting is a problem. In overfitting, the model learns too much about the training data and is unable to generalise its learnings for unseen data which leads to poor performance on new data points.]** . We first analyse the given example and discuss the probable causes of the underlying problem. Then we investigate how the depth and width of a neural network can affect overfitting in a feedforward architecture and observe that increasing width and depth **[Question 2 - Summarise the effect increasing width and depth of the architecture had on overfitting. Increaseing the depth and width slightly increases the model performance overall but if the either or both the width and depth are increased by a lot, the model overfits the training data and returns low accuracy scores for the validation set.]** . Next we discuss how two standard methods, Dropout and Weight Penalty, can mitigate overfitting, then describe their implementation and use them in our experiments to reduce the overfitting on the EMNIST dataset. Based on our results, we ultimately find that **[Question 3 - Summarise what your results show you about the effect of the tested approaches on overfitting and the performance of the trained model]** . Finally, we conclude the report with our observations and related work. Our main findings indicate that **[Question 4 - Give your overall conclusions]** .

1. Introduction

In this report we focus on a common and important problem while training machine learning models known as overfitting, or overtraining, which is the training regime where performances increase on the training set but decrease on unseen data. We first start with analysing the given problem in Figure 1, study it in different architectures and then investigate different strategies to mitigate the problem. In particular, Section 2 identifies and discusses the given problem, and investigates the effect of network width and depth in terms of generalisation gap (see Ch. 5 in Goodfellow et al. 2016) and generalisation performance. Section 3 introduces two regularisation techniques to alleviate overfitting: Dropout (Srivastava et al., 2014) and L1/L2 Weight Penalties (see Section 7.1 in Goodfellow et al. 2016). We first explain them in detail and discuss why they are used for alleviating overfitting. In Section 4, we incorporate each of them and their various combinations to a three hidden layer[1] neural network, train it on the EMNIST dataset, which contains 131,600 images of characters and digits, each of size 28x28, from 47 classes. We evaluate them in terms of generalisation gap and performance, and discuss the results and effectiveness of the tested regularisation strategies. Our results show that **[Question 3 - Summarise what your results show you about the effect of the tested approaches on overfitting and the performance of the trained model]** .

Finally, we conclude our study in Section 5, noting that **[Question 4 - Give your overall conclusions]** .

2. Problem identification

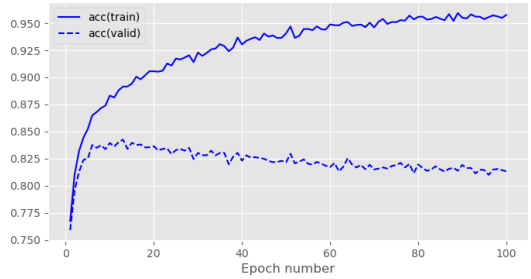
Overfitting to training data is a very common and important issue that needs to be dealt with when training neural networks or other machine learning models in general (see Ch. 5 in Goodfellow et al. 2016). A model is said to be overfitting when as the training progresses, its performance on the training data keeps improving, while its is degrading on validation data. Effectively, the model stops learning related patterns for the task and instead starts to memorize specificities of each training sample that are irrelevant to new samples.

[Question 5 - Explain in detail, and in your own words, why overfitting is a problem] .

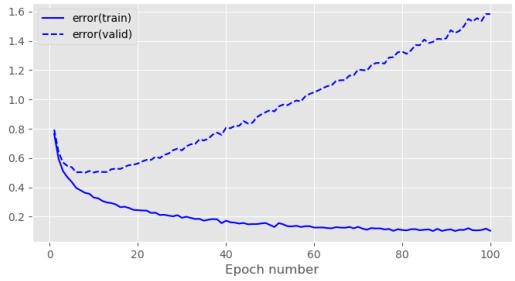
Although it eventually happens to all gradient-based training, it is most often caused by models that are too large with respect to the amount and diversity of training data. The more free parameters the model has, the easier it will be to memorise complex data patterns that only apply to a restricted amount of samples. A prominent symptom of overfitting is the generalisation gap, defined as the difference between the validation and training error. A steady increase in this quantity is usually interpreted as the model entering the overfitting regime.

[Question 6 - Explain the relevance of "network capacity" to overfitting] .

[1] We denote all layers as hidden except the final (output) one. This means that depth of a network is equal to the number of its hidden layers + 1.



(a) accuracy by epoch



(b) error by epoch

Figure 1. Training and validation curves in terms of classification accuracy (a) and cross-entropy error (b) on the EMNIST dataset for the baseline model.

# Hidden Units	Val. Acc.	Train Error	Val. Error
32	–.-	-.—	-.—
64	–.-	-.—	-.—
128	–.-	-.—	-.—

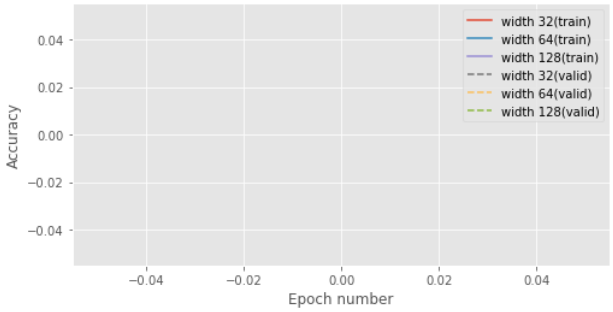
Table 1. Validation accuracy (%) and training/validation error (in terms of cross-entropy error) for varying network widths on the EMNIST dataset.

Figure 1a and 1b show a prototypical example of overfitting. We see in Figure 1a that **[Question 7 - Explain what these figures contain and how the curves evolve, and spot where overfitting occurs. Reason based on the min/max points and velocities (direction and magnitude of change) of the accuracy and error curves]** .

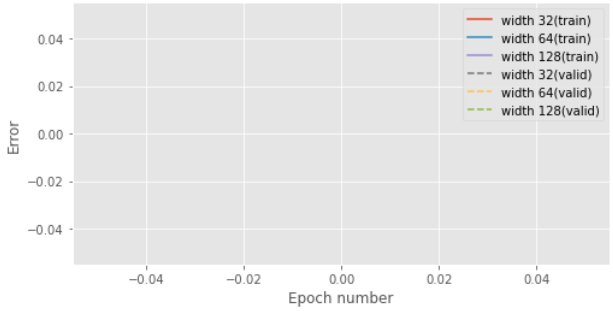
The extent to which our model overfits depends on many factors. For example, the quality and quantity of the training set and the complexity of the model. If we have sufficiently many diverse training samples, or if our model contains few hidden units, it will in general be less prone to overfitting. Any form of regularisation will also limit the extent to which the model overfits.

2.1. Network width

[Question Table 1 - Fill in Table 1 with the results from your experiments varying the number of hidden units.] [Question Figure 2 - Replace the images in Figure 2 with figures depicting the accuracy and error, training and validation curves for your experiments varying the number of hidden units.]



(a) accuracy by epoch



(b) error by epoch

Figure 2. Training and validation curves in terms of classification accuracy (a) and cross-entropy error (b) on the EMNIST dataset for different network widths.

First we investigate the effect of increasing the number of hidden units in a single hidden layer network when training on the EMNIST dataset. The network is trained using the Adam optimiser with a learning rate of 9×10^{-4} and a batch size of 100, for a total of 100 epochs.

The input layer is of size 784, and output layer consists of 47 units. Three different models were trained, with a single hidden layer of 32, 64 and 128 ReLU hidden units respectively. Figure 2 depicts the error and accuracy curves over 100 epochs for the model with varying number of hidden units. Table 1 reports the final accuracy, training error, and validation error. We observe that **[Question 8 - Present your network width experiment results by using the relevant figure and table]** .

[Question 9 - Discuss whether varying width affects the results in a consistent way, and whether the results are expected and match well with the prior knowledge (by which we mean your expectations as are formed from the relevant Theory and literature)] .

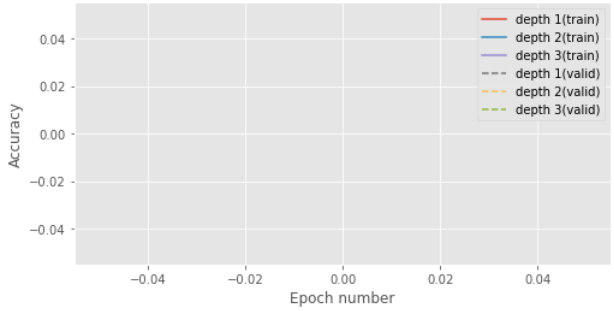
2.2. Network depth

[Question Table 2 - Fill in Table 2 with the results from your experiments varying the number of hidden layers.] [Question Figure 3 - Replace these images with figures depicting the accuracy and error, training and validation curves for your experiments varying the number of hidden layers.]

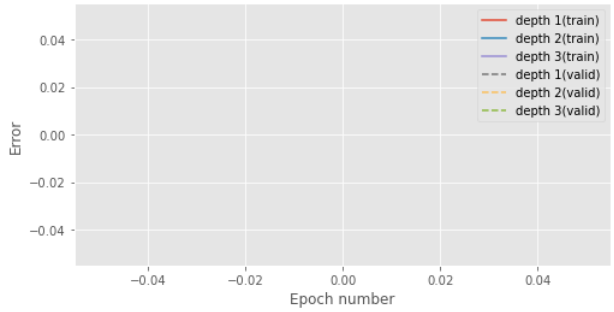
Next we investigate the effect of varying the number of

# Hidden Layers	Val. Acc.	Train Error	Val. Error
1	–.-	-.—	-.—
2	–.-	-.—	-.—
3	–.-	-.—	-.—

Table 2. Validation accuracy (%) and training/validation error (in terms of cross-entropy error) for varying network depths on the EMNIST dataset.



(a) accuracy by epoch



(b) error by epoch

Figure 3. Training and validation curves in terms of classification accuracy (a) and cross-entropy error (b) on the EMNIST dataset for different network depths.

hidden layers in the network. Table 2 and Figure 3 depict results from training three models with one, two and three hidden layers respectively, each with 128 ReLU hidden units. As with previous experiments, they are trained with the Adam optimiser with a learning rate of 9×10^{-4} and a batch size of 100.

We observe that **[Question 10 - Present your network depth experiment results by using the relevant figure and table]** .

[Question 11 - Discuss whether varying depth affects the results in a consistent way, and whether the results are expected and match well with the prior knowledge (by which we mean your expectations as are formed from the relevant Theory and literature)] .

3. Dropout and Weight Penalty

In this section, we investigate three regularisation methods to alleviate the overfitting problem, specifically dropout layers and the L1 and L2 weight penalties.

3.1. Dropout

Dropout (Srivastava et al., 2014) is a stochastic method that randomly inactivates neurons in a neural network according to an hyperparameter, the inclusion rate (*i.e.* the rate that an unit is included). Dropout is commonly represented by an additional layer inserted between the linear layer and activation function. Its forward pass during training is defined as follows:

$$\text{mask} \sim \text{bernoulli}(p) \tag{1}$$

$$\boldsymbol{y}' = \text{mask} \odot \boldsymbol{y} \tag{2}$$

where $\boldsymbol{y}, \boldsymbol{y}' \in \mathbb{R}^d$ are the output of the linear layer before and after applying dropout, respectively. mask $\in \mathbb{R}^d$ is a mask vector randomly sampled from the Bernoulli distribution with inclusion probability p, and $\odot$ denotes the element-wise multiplication.

At inference time, stochasticity is not desired, so no neurons are dropped. To account for the change in expectations of the output values, we scale them down by the inclusion probability p:

$$\boldsymbol{y}' = \boldsymbol{y} * p \tag{3}$$

As there is no nonlinear calculation involved, the backward propagation is just the element-wise product of the gradients with respect to the layer outputs and mask created in the forward calculation. The backward propagation for dropout is therefore formulated as follows:

$$\frac{\partial \boldsymbol{y}'}{\partial \boldsymbol{y}} = mask \tag{4}$$

Dropout is an easy to implement and highly scalable method. It can be implemented as a layer-based calculation unit, and be placed on any layer of the neural network at will. Dropout can reduce the dependence of hidden units between layers so that the neurons of the next layer will not rely on only few features from of the previous layer. Instead, it forces the network to extract diverse features and evenly distribute information among all features. By randomly dropping some neurons in training, dropout makes use of a subset of the whole architecture, so it can also be viewed as bagging different sub networks and averaging their outputs.

3.2. Weight penalty

L1 and L2 regularisation (Ng, 2004) are simple but effective methods to mitigate overfitting to training data. The application of L1 and L2 regularisation strategies could be formulated as adding penalty terms with L1 and L2 norm square of weights in the cost function without changing other formulations. The idea behind this regularisation method is to penalise the weights by adding a term to the cost function, and explicitly constrain the magnitude of the weights with either the L1 and L2 norms. The optimisation

problem takes a different form:

$$\text{L1: } \min_{\boldsymbol{w}} E_{\text{data}}(\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{w}) + \lambda ||w||_1 \quad (5)$$

$$\text{L2: } \min_{\boldsymbol{w}} E_{\text{data}}(\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{w}) + \lambda ||w||_2^2 \quad (6)$$

where E_{data} denotes the cross entropy error function, and $\{\boldsymbol{X}, \boldsymbol{y}\}$ denotes the input and target training pairs. λ controls the strength of regularisation.

Weight penalty works by constraining the scale of parameters and preventing them to grow too much, avoiding overly sensitive behaviour on unseen data. While L1 and L2 regularisation are similar to each other in calculation, they have different effects. Gradient magnitude in L1 regularisation does not depend on the weight value and tends to bring small weights to 0, which can be used as a form of feature selection, whereas L2 regularisation tends to shrink the weights to a smaller scale uniformly.

[Question 12 - Explain how one could use a combination of L1 and L2 regularisation. Discuss any potential benefits of this approach] .

4. Balanced EMNIST Experiments

[Question Table 3 - Fill in Table 3 with the results from your experiments for the missing hyperparameter values for each of L1 regularisation, L2 regularisation, and Dropout (use the values shown on the table).]

[Question Figure 4 - Replace these images with figures depicting the Validation Accuracy and Generalisation Gap (difference between validation and training error) for each of the experiment results varying the Dropout inclusion rate, and L1/L2 weight penalty depicted in Figure 3 (including any results you have filled in).]

Here we evaluate the effectiveness of the given regularisation methods for reducing the overfitting on the EMNIST dataset. We build a baseline architecture with three hidden layers, each with 128 neurons, which suffers from overfitting as shown in section 2.

Here we train the network with a lower learning rate of 10^{-4}, as the previous runs were overfitting after only a handful of epochs. Results for the new baseline (c.f. Table 3) confirm that lower learning rate helps, so all further experiments are run using it.

Then, we apply the L1 or L2 regularisation with dropout to our baseline and search for good hyperparameters on the validation set. We summarise all the experimental results in Table 3. For each method, we plot the relationship between generalisation gap and validation accuracy in Figure 4.

First we analyze three methods separately, train each over a set of hyperparameters and compare their best performing results.

[Question 13 - Explain the experimental details (e.g. hyperparameters), discuss the results in terms of their generalisation performance and overfitting. Select and test the best performing model as part of this analysis.] .

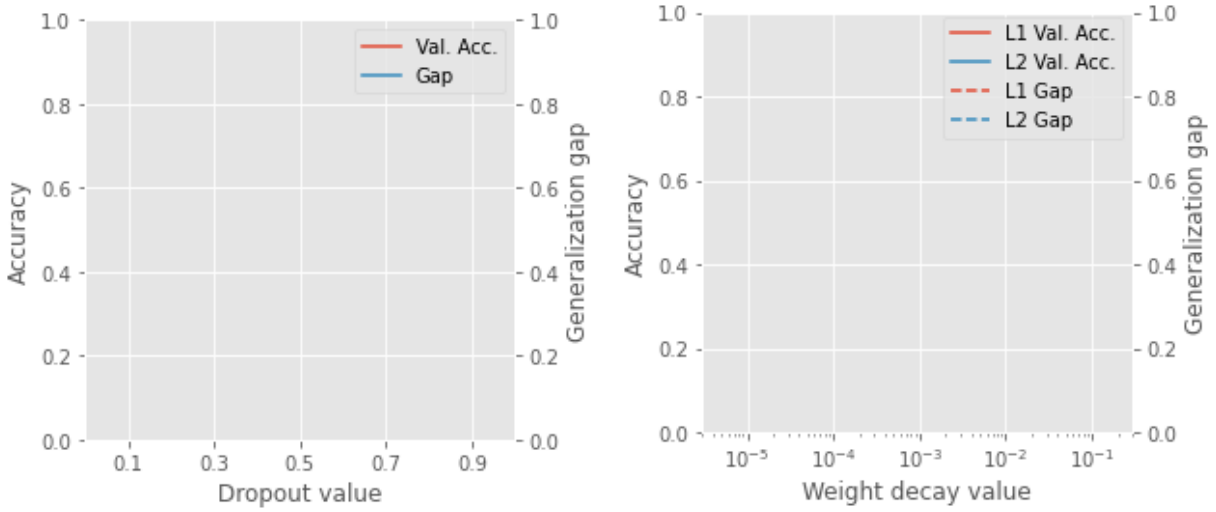
[Question 14 - Assume you were able to run 8 further experiments (8 specific hyperparameter configurations) where you could combine Dropout and L1, and/or Dropout and L2 regularisation. Which 8 runs would you pick and what question(s) would you aim to answer? Make sure you define the experiment setup, including any relevant hyperparameters] .

5. Conclusion

[Question 15 - Briefly draw your conclusions based on the results from the previous sections (what are the take-away messages?), discussing them in the context of the overall literature, and conclude your report with a recommendation for future directions] .

Model	Hyperparameter value(s)	Validation accuracy	Train Error	Validation Error
Baseline	-	0.837	0.241	0.533
Dropout	0.6	80.7	0.549	0.593
	0.7	–.-	-.—	-.—
	0.85	85.1	0.329	0.434
	0.97	85.4	0.244	0.457
L1 penalty	5e-4	79.5	0.642	0.658
	1e-3	–.-	-.—	-.—
	5e-3	2.41	3.850	3.850
	5e-2	2.20	3.850	3.850
L2 penalty	5e-4	85.1	0.306	0.460
	1e-3	–.-	-.—	-.—
	5e-3	81.3	0.586	0.607
	5e-2	39.2	2.258	2.256

Table 3. Results of all hyperparameter search experiments. *italics* indicate the best results per series (Dropout, L1 Regularisation, L2 Regularisation) and **bold** indicates the best overall.



(a) Accuracy and error by inclusion probability.

(b) Accuracy and error by weight penalty.

Figure 4. Accuracy and error by regularisation strength of each method (Dropout and L1/L2 Regularisation).

References

Goodfellow, Ian, Bengio, Yoshua, and Courville, Aaron. *Deep Learning*. MIT Press, 2016. http://www.deeplearningbook.org.

Ng, Andrew Y. Feature selection, l1 vs. l2 regularization, and rotational invariance. In *Proceedings of the twenty-first international conference on Machine learning*, pp. 78, 2004.

Srivastava, Nitish, Hinton, Geoffrey, Krizhevsky, Alex, Sutskever, Ilya, and Salakhutdinov, Ruslan. Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research*, 15(1): 1929–1958, 2014.