
MLP Coursework 1

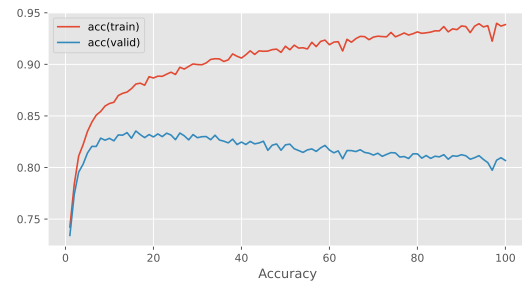
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Abstract

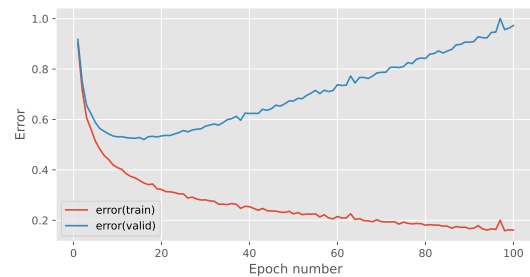
In this report we study the problem of overfitting, which is [when a network function is too closely fit to a training set, and results in an increasing validation set error despite a monotonically decreasing training error(an illustration of this concept is shown in figure 1b).] . We first analyse the 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] . Next we discuss why 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 briefly review another method, Maxout, discuss its strengths and weaknesses, and conclude the report with our observations and future 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 [when a network function is too closely fit to a training set, and results in an increasing validation set error despite a monotonically decreasing training error(an illustration of this concept is shown in figure 1b).] . We first start with analyzing the given problem in Fig. 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 generalization gap (see Ch. 5 in Goodfellow et al. 2016) and generalization performance. Section 3 introduces two regularization 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



(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.

of them and their various combinations to a three hidden layer neural network, train it on the EMNIST dataset, which contains 131,600 images of characters and digits, each of size 28x28 which are split into 47 classes, grouping together some difficult to distinguish characters. We evaluate them in terms of generalization gap and performance, and discuss the results and effectiveness of the tested regularization 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] . In Section 5, we discuss a related work on Maxout Networks and highlight its pros and cons.¹ Finally, we conclude our study in section 6, 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

¹Instructor note: Omitting this for this coursework, but normally you would be more specific and summarise your conclusions about that review here as well.

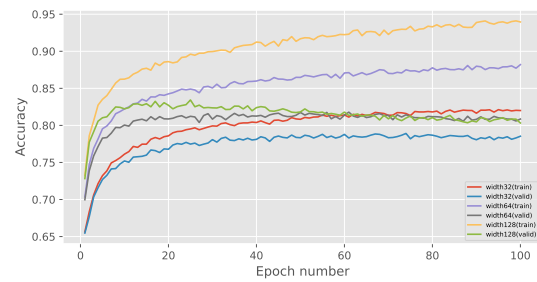
networks or other machine learning models in general (see Ch. 5 in Goodfellow et al. 2016). A model is said to be overfitting when [it's validation error begins to increase despite it's training error decreasing monotonically. This leads to an increasing generalization gap as the model is trained over a number of epochs. It indicates that the model is too flexible and doesn't fit to unseen data very well.] .

[Overfitting occurs due to a high variance being present within the trained model. This is due to the model becoming overly complex and fitting its degrees of freedom in such a way which closely resembles data points present in the training data. The parameters of the model learn the detail and noise in the training data which results in a negative performance when it comes to the generalization of the model and its ability to closely predict outputs on unseen data. Overfitting can occur for a number of reasons. If the learning rate of a model is increased too much, then it is likely that the parameters of the model will converge and resemble training data points very closely in a fewer number of epochs respectively. A clear way to identify if a model is overfit is by visualising the error of the model on a training and validation set across a fixed number of epochs. If the validation error begins to increase despite a monotonically decreasing training error, the model is said to be overfitted. To generalize, if the Model performs well on a training set, but poorly on unseen data, it is overfitted.] .

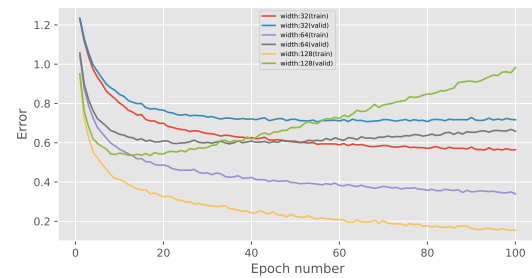
Fig. 1a and 1b show a prototypical example of overfitting. We see in Figure 1a that [it highlights the ratio of total EMNIST samples which were classified with their target labels correctly over a period of 100 epochs. the red and blue lines represent the accuracy obtained by the baseline model across the training and test set respectively. It can be observed that the accuracy of predictions steeply increased up until epoch 5. Beyond which training accuracy continued to increase steeply in contrast to the validation accuracy which increased at a slower rate and began to level off. At around epoch 16, it is clear that the model was no longer improving in validation accuracy due to a flat gradient in the validation accuracy curve. This indicates a maximum optimum accuracy of 82.5% was achieved for the model at epoch 16 before it's performance began to decline. Figure 1b similarly illustrates epoch 16 as the point where the cross-entropy error measured on the validation set was at it's minimum of 0.5, before it began to increase. It can be deduced that beyond epoch 16, training accuracy continued to increase monotonically, whereas validation accuracy began to decline. A similar pattern can be observed for figure 1b where the error on the training set continued to decrease beyond epoch 16, whereas it increased for the validation set. This led to an expanding generalization gap. Hence, the baseline model became overfitted beyond epoch 16. By the end of epoch 100, it can be seen that the accuracy across

# hidden units	val. acc.	generalization gap
32	78.5	0.15
64	80.9	0.32
128	80.3	0.83

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



(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.

the validation set had fallen from 82.5% to 80.5%. Furthermore, the error across the validation set increased from a minimum of 0.5 to approximately 0.98. In contrast, by epoch 100, the training set was clearly fitted to the model due to the high training accuracy of 93.5% and low error of 0.17.] .

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 a lot of varied training samples, or if our model is relatively shallow, 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.]

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 optimizer with a learning rate of 10^{-3} 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 and generalization gap. We observe that [as the number of hidden units is increased, this does lead to an improvement in validation accuracy, as shown in table 1. The final validation accuracy increased from 78.5% for 32 units to 80.3% for 128 units. We observe that the highest final validation accuracy of 80.9% was achieved using 64 hidden units. The reason why the 128 unit model was unable to outperform the 64 units model is due to overfitting. Figure 2a and 2b shows that overfitting of the 128 model is indicated by the rise in validation error (green line) beyond epoch 18, despite its corresponding training error decreasing (yellow line). This led to the decrease in validation accuracy as shown in figure 2a for accuracies recorded beyond epoch 18. By the end of epoch 100, we can see that the 64 units model performed almost identically to the 128 units model on the validation set. The 128 units model had an advantage when it comes to how quickly the model converged and obtained lower validation error and higher validation accuracies. It achieved a maximum validation accuracy of approximately 82.5% after epoch 18. It was also the fastest model to see a drastic improvement in validation accuracy. However due to overfitting, this advantage didn't last too long. The 32 layer model performed the worst on the validation set and obtained the lowest accuracy across the board. This is due to the model being underfit and not flexible enough to learn the parameters needed to fit the training data well. Despite this, it did obtain the lowest generalization error of 0.15 so is the least likely model to result in overfitting. In contrast, the 128 unit model is the most likely to overfit due to a high generalization gap of 0.83.]

[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.]

# hidden layers	val. acc.	generalization gap
1		
2		
3		

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

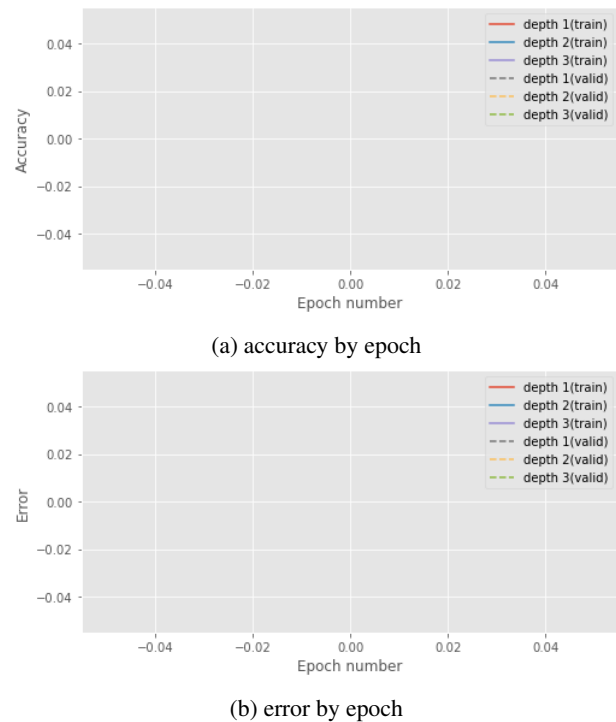


Figure 3. Training and validation curves in terms of classification accuracy (a) and cross-entropy error (b) on the EMNIST dataset for different network depths.

Next we investigate the effect of varying the number of hidden layers in the network. Table 2 and Fig. 3 shows the 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 optimizer with a learning rate of 10^{-3} and a batch size of 100.

We observe that [Question 10 - Explain 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)]

[Question 12 - Compare and discuss how varying width and height changes the performance and overfitting in your experiments]

3. Dropout and Weight Penalty

In this section, we investigate three regularization 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. Dropout is commonly represented by an additional layer inserted between the linear layer and activation function. Its forward propagation during training is defined as follows:

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

$$y' = mask \odot y \quad (2)$$

where $y, y' \in \mathbb{R}^d$ 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 parameter of 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 rate p :

$$y' = y * p \quad (3)$$

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:

$$\frac{\partial y'}{\partial y} = mask \quad (4)$$

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 features between layers so that the neurons of the next layer will not specifically depend on some features from of the previous layer. Instead, it force the network to 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 regularization (Ng, 2004) are simple but effective methods to mitigate overfitting to training data. [Question

13 - Explain L1/L2 weight penalties first in words and then with formulas. Explain how they are incorporated to training and what hyperparameter(s) they require] .

[Question 14 - Discuss how/why the weight penalties may address overfitting, discuss how L1 and L2 regularization differ and support your claims with references where possible] .

4. Balanced EMNIST Experiments

[Question Table 3 - Fill in Table 3 with the results from your experiments varying the hyperparameter values for each of L1 regularisation, L2 regularisation, and Dropout (use the values shown on the table) as well as the results for your experiments combining L1/L2 and Dropout (you will have to pick what combinations of hyperparameter values to test for the combined experiments; each of the combined experiments will need to use Dropout and either L1 or L2 regularisation; run an experiment for each of 8 different combinations). Use *italics* to print the best result per criterion for each set of experiments, and bold for the overall best result per criterion.]

[Question Figure 4 - Replace these images with figures depicting the Validation Accuracy and Generalisation Gap for each of your experiments varying the Dropout inclusion rate, L1/L2 weight penalty, and for the 8 combined experiments (you will have to find a way to best display this information in one subfigure).]

Here we evaluate the effectiveness of the given regularization 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 in EMNIST as shown in section 2.

We start by lowering the learning rate to 10^{-4} , as the previous runs were overfitting in only a handful of epochs. Results for the new baseline (c.f. Table 3) confirm that lowering learning rate helps, so all further experiments are run using it.

Then, we apply the L1 or L2 regularization with dropout to our baseline and search for good hyperparameters on the validation set. We summarize 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 15 - Explain the experimental details (e.g. hyperparameters), discuss the results in terms of their generalization performance and overfitting] .

5. Literature Review: Maxout Networks

Summary of Maxout Networks In this section, we briefly discuss another generalization method: Maxout net-

Model	Hyperparameter value(s)	Validation accuracy	Generalization gap
Baseline	-	0.836	0.290
Dropout	0.7		
	0.9		
	0.95		
L1 penalty	1e-4		
	1e-3		
	1e-1		
L2 penalty	1e-4		
	1e-3		
	1e-1		
Combined	for example 0.95, L1 1e-6		
	?, ?		
	?, ?		
	?, ?		
	?, ?		
	?, ?		

Table 3. Results of all hyperparameter search experiments. *italics* indicate the best results per series and **bold** indicate the best overall

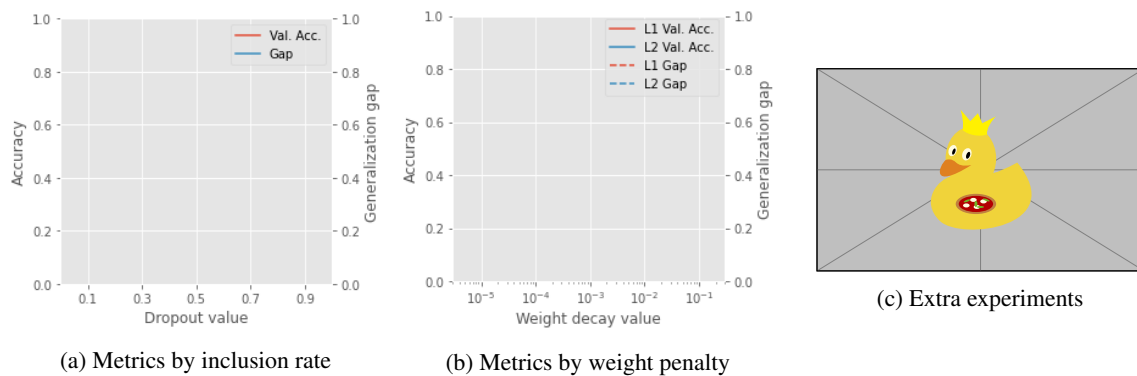


Figure 4. Hyperparameter search for every method and combinations

works (Goodfellow et al., 2013). This paper further explores the dropout method and proposes a new "maxout" layer which can complement dropout. The authors evaluate the performance of Maxout Networks in four standard datasets, namely MNIST, CIFAR-10 and 100, and SVHN. They point out that although dropout has been widely applied in deep models, [Question 16 - Explain the motivation behind Maxout Networks as presented in (Goodfellow et al., 2013)]. Following this motivation, they propose the Maxout activation layers. These can be considered learnable activations that work as a universal convex function approximator. The Maxout layer first maps the hidden space to k subspaces through independent affine transformations, then, for each element in output vectors, it takes the maximum value across all subspaces.

[Question 17 - State whether Dropout is compatible (can be used together) with Maxout and explain why].

Strengths and limitations The author proposed a novel neural activation unit that further exploits the dropout technique. [Question 18 - Give an overview of the exper-

iment setup in (Goodfellow et al., 2013) and analyse it from the point of view of how convincing their conclusions are].

Although the Maxout activation units can maximize the averaging effect of dropout in a deep architecture, we can argue that the Maxout computation is expensive. The advantage of dropout lies in its high scalability and computational advantages. It can be arbitrarily applied to various network structures, and the calculation speed is fast, which is very suitable for heavy computing algorithms such as training and inference of neural networks. In comparison, the design of the Maxout network needs to project the hidden vector into k subspaces. Both the forward algorithm and the backward algorithm of dropout can be calculated in $O(D)$ complexity, but the complexity of Maxout is $O(kD)$. This can lead to increasing the number of training epochs needed to reach convergence. Furthermore, the universal approximation property of Maxout seems powerful, but it would be interesting to verify that it is useful in practice. Specifically, we can design an experiment where we increase the number of subspaces k and see where performances stop

improving. In extreme cases, it is even possible that the function learned is too specific to the training data, effectively causing overfitting.

6. Conclusion

[Question 19 - Briefly draw your conclusions based on the results from the previous sections (what are the take-away messages?) and conclude your report with a recommendation for future directions] .

References

- Goodfellow, Ian, Warde-Farley, David, Mirza, Mehdi, Courville, Aaron, and Bengio, Yoshua. Maxout networks. In *International conference on machine learning*, pp. 1319–1327. PMLR, 2013.
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