# 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. **[When overfitting occurs, the model can only be able to fit well on the training set(we do have labels/results) and unable to generalize well to new data(we do not know, results to be discovered). So the model can not perform the classification or prediction tasks that it was intended for]** . 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 a technique that studies use of weight decay in adaptive gradient algorithms, discuss its findings, 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 the training regime where performances increase on the training set but decrease on unseen data. 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 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 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 study a related work that studies weight decay in adaptive gradient algorithms.[2] Finally, we conclude our study in section 6, noting that **[Question 4 - Give your overall conclusions]** .

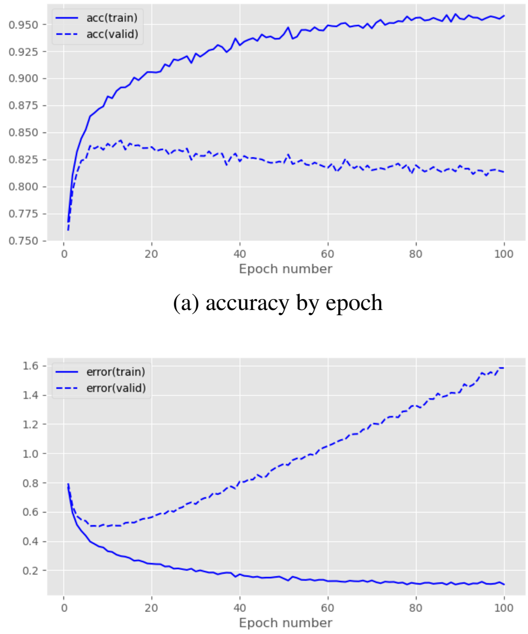
## 2. Problem identification

Overfitting to training data is a very common and important issue that needs to be dealt with when training neural 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.

**[Since the goal of the model is to extract of the commonalities of some classes from the training set, and use these commonalities to do prediction or classification on new data(same distribution as training set). While overfitting leads the model to memorizing too many details(like the outliers, or small disturbances due to noise), which results in a more complex model and weakens generalization of data commonalities in general. For example, considering the task of human identification intuitively. If the "real" human in training set all wear red clothes. When overfitting occurs, although the model can correctly recognize almost every person in training set, it may classify a naked person(in new data set) as non-human, despite the person has enough commonality with "real" human. For the model remembers more commonalities than the model without overfitting do]** .

[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.

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



(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.

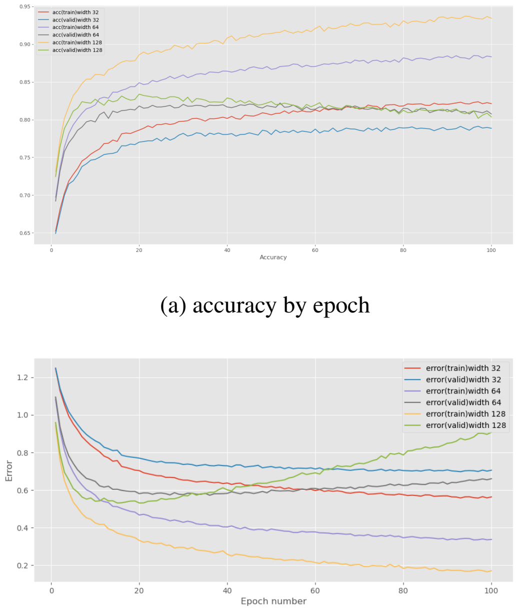
Although it eventually happens to all gradient-based training, it is most often caused by models that are too large with respect to the amount and diversity of training data. The more free parameters the model has, the easier it will be to memorize complex data patterns that only apply to a restricted amount of samples. A prominent symptom of overfitting is the generalization 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]** .

Fig. 1a and 1b show a prototypical example of overfitting. We see in Fig. 1a that **[The Fig.1a contains the accuracy(training and validation) by epoch and the Fig.1b contrains the error(training and validation)by epoch, the the range of epoch is from 0 to 100. In Fig.1a, the training accuracy increases fast before epoch 10 and after that it increases more slowly and get to the peak of about 0.950 at epoch 90. The validation accuracy increases at the beginning of training and reaches the maximum of 0.835 at around epoch 10. After epoch 10 the validation continuous to decline to 0.810. In Fig.1b, the training error decreases fast before epooch 10 and after that it decreases more slowly and get to the minimum of about 0.05 at epoch 90. The validation error decreases and get to the minimum of 0.5 at epoch 10. After epoch 10, the validation error grows almost linearly with respect to epoch and grows rapidly]** .

| # Hidden Units | Val. Acc. | Train Error | Val. Error |
|---|---|---|---|
| 32 | 0.789 | 0.563 | 0.705 |
| 64 | 0.808 | 0.337 | 0.660 |
| 128 | 0.804 | 0.170 | 0.907 |

*Table 1.* Validation accuracy (%) and training/validation error (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 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

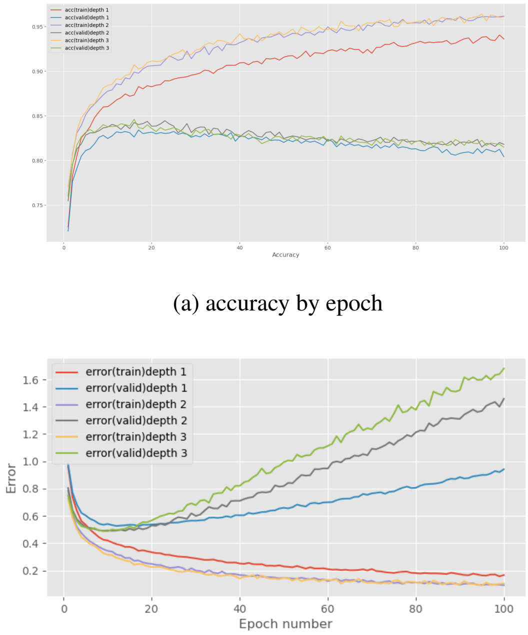
**[ Question Table 1 - Fill in Table 1 with the results from your experiments varying the number of hidden units. ] [Question Figure 2 - Replace the images in Figure 2 with figures depicting the accuracy and error, training and validation curves for your experiments varying the number of hidden units.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

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 $9 \times 10^{-4}$ 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

| # Hidden Layers | Val. Acc. | Train Error | Val. Error |
|---|---|---|---|
| 1 | 0.804 | 0.167 | 0.942 |
| 2 | 0.818 | 0.0925 | 1.46 |
| 3 | 0.815 | 0.105 | 1.68 |

*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.

single hidden layer of 32, 64 and 128 ReLU hidden units respectively. Fig. 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 - Explain 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 in the network. Table 2 and Fig. 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 optimizer with a learning rate of $9 \times 10^{-4}$ 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 (*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:

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

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 regularization (Ng, 2004) are simple but effective methods to mitigate overfitting to training data. The application of L1 and L2 regularization 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 regularization method is to penalize 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 optimization problem takes a different form:

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

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

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

Weight penalty works by constraining the scale of parameters and preventing them to grow too much, avoiding overly sensitive behavior on unseen data. While L1 and L2 regularization are similar to each other in calculation, they have different effects. Gradient magnitude in L1 regularization 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 regularization tends to shrink the weights to a smaller scale uniformly.

**[Question 13 - Explain how one could use a combination of L1 and L2 regularization. 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 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 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 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 14 - Explain the experimental details (e.g. hyperparameters), discuss the results in terms of their generalization performance and overfitting. Select and test the best performing model as part of this analysis]** .

**[Question 15 - Assume you were able to run 8 further experiments where you could combine Dropout and L1, and/or Dropout and L2 regularization. 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. Literature Review: Decoupled Weight Decay Regularization

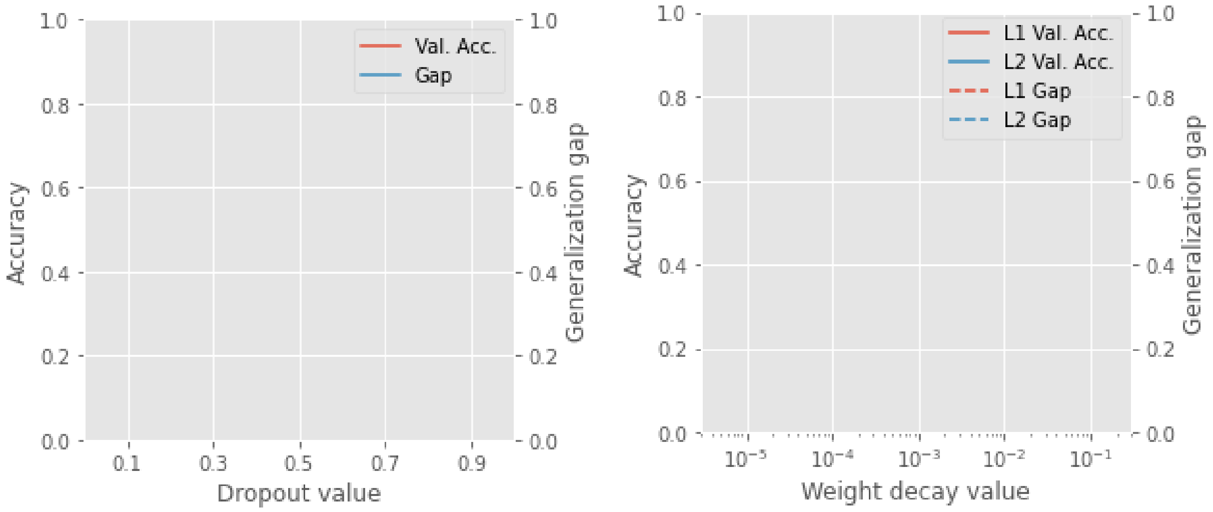
**Summary** In this section, we briefly study a method (Loshchilov & Hutter, 2019) that decouples the weight penalty from the weight update. The authors shed light onto the relation between weight decay and L2 weight penalty for SGD and Adam optimizers, pointing out that weight decay and L2 weight penalty are not equivalent when used with the Adam optimizer.

In particular, the authors claim that SGD with L2 weight penalty and weight decay are equivalent when their coefficients have the relation $\lambda' = \frac{\lambda}{\alpha}$ (see their **Proposal 1**), which they prove with Equations (5) and (6) (proof is in their Appendix A). In addition, they claim that such a simple scalar relation does not hold in Adam optimization (see **Proposal 2**) and show, in their Appendix A, that the necessary relation for equivalence requires use of a preconditioner matrix $\boldsymbol{M}_t$. This requirement can be explained with the fact that **[Question 16 - Explain, in your own words, why the equivalence between L2 weight penalty and weight decay in Adam optimizer requires a more complex relation; a preconditioner matrix $M_t$ rather than a scalar relation]** .

**[Question 17 - Based on Algorithm 2 in (Loshchilov & Hutter, 2019), discuss whether your code with L2 Weight Penalty in the MLP library implements "Adam**

| 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 Regularization, L2 Regularization) 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 regularization strength of each method (Dropout and L1/L2 Regularization).

**with L2 regularization”, “Adam with decoupled weight decay (AdamW)” or another variation. Refer to the MLP code, pointing to the specific files and functions to justify your answer]** .

Finally the authors validate their findings and proposed decoupled optimization strategies in various learning rate schedules, initial learning rates, network architectures and datasets. [3]

## 6. Conclusion

**[Question 18 - 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]** .

[3] Instructor note: Omitting this for this coursework, but normally you would give an evaluation of the experiment setup in (Loshchilov & Hutter, 2019) here.

## References

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

Loshchilov, Ilya and Hutter, Frank. Decoupled weight decay regularization. In *International Conference on Learning Representations (ICLR)*, 2019.

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.