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Implementation and Optimisation of a Neural Network

How stepping schedules affect learning

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Abstract

As this project covers an implementation and optimisation of a neural network, it covers most of the essentials within the field of neural networks and its place within machine learning. The focus, however, lay on studying how stepping schedules affect learning. A stepping schedule is a predetermined way to decrease the learning rate over the training process. It turns out that for the networks implemented, stepping schedules do *not* seem to make a significant difference in performance, although slight improvements from constant learning rates could be found in some cases. Even when different depths and widths of the neural network were studied, a stepping schedule did not seem to have much of an impact. This result is somewhat surprising, as we in theory would expect to see a rise in performance when the learning rate is gradually decreased over learning. We can conclude that other correctly chosen parameters play a much more significant role in facilitating an effective learning process. The code of the implementation is found through the following link `https://github.com/axeboii/Neural-Network`.

Sammanfattning

Eftersom detta projekt omfattar en implementering och optimering av ett neuralt nätverk, täcker rapporten det mest väsentliga inom neurala nätverk och dess plats inom området maskininlärning. Fokus ligger dock på att studera hur stegscheman påverkar inlärning. Ett stegschema är ett på förhand bestämt sätt att minska inlärningshastigheten (learning rate) under träningsprocessen. Det visar sig att för de implementerade nätverken verkar stegscheman *inte* göra någon signifikant skillnad i prestanda, även om små förbättringar från konstanta inlärningshastigheter kunde ses i vissa fall. Även när olika djup och bredd på det neurala nätverket studerades verkade stegscheman inte ha någon större påverkan på inlärningen. Detta resultat är något överraskande, eftersom vi i teorin borde kunna förvänta oss en ökning i prestanda när inlärningshastigheten gradvis minskar under inlärningen. Vi kan dra slutsatsen att andra korrekt valda parametrar spelar en mycket viktigare roll för en effektiv inlärningsprocess. Koden för implementationen finns via följande länk `https://github.com/axeboii/Neural-Network`.

Preface

This report was written as part of a bachelor's degree project in Vehicle Engineering at KTH, Royal Institute of Technology, Stockholm, Sweden. Before entering into this project we had no previous experience in the field of machine learning in general or neural networks in particular. Realising that there may be some new terminology introduced to the reader, we recommend keeping an eye on the word list found in appendix 7.1 for brief explanations of concepts. We hope that you will find the report interesting.

Axel Boivie & Victor Bellander, Stockholm, May 2021

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1 Introduction

In today's society, machine learning plays an increasingly important role. Classification is an important machine learning task, whether it regards speech recognition, face detection, document classification or in the case of this project, handwriting recognition. A neural network is a machine learning algorithm well suited for such a task. In this project, a neural network will be implemented, trained and tested with labelled handwritten digits (MNIST dataset). The goal is to study how stepping schedules implemented in stochastic gradient descent can help optimise training. A stepping schedule is a beforehand determined scheme to decrease the learning rate over a training process, which can help maximising progress in training. If you are unfamiliar with these terms, they will be explained in much further detail shortly. A challenge for neural networks today is optimising training, as accurate networks with reasonable computational demands are desirable. This is especially important in smaller or mobile units, where energy and computational capacity is limited. Hopefully, a stepping schedule could help achieving this. A more rigorous account of the issue dealt with in this report is presented in section 1.2.

1.1 Background

As the field of neural networks is so comprehensive, this background section focuses on theory related to the implementation of a neural network from scratch in python with the objective of classifying images.

1.1.1 Neural networks

A neural network (NN) is a complex type of machine-learning algorithm. The name comes from its resemblance to a biological neural network, such as those found in our brains where neuron cells are linked together. Similarly, a neural network consists of nodes linked together in a network-like fashion. The idea is that these nodes are organised in layers, with an input layer, an arbitrary number of hidden layers and an output layer. These layers consist of several nodes, which all have connections to the next layer. As the number of layers and nodes within them increases, we reach what is commonly known as *deep learning*. There are too many types of neural network structures for this report to handle, so this report is limited to fully connected neural networks. This means that every node at a specific layer is connected to all nodes at the next layer. Networks in this report will rely on supervised learning, meaning all training data are labelled with its correct answer. (Goodfellow et. al, 2016)

In a mathematical way, a general neural network can be described as a function $\mathbf{f}(\mathbf{x};\boldsymbol{\theta}) : \mathbb{R}^m \to \mathbb{R}^n$, where $\mathbf{x}$ is the input to the function, $\mathbf{f}$ the output and $\boldsymbol{\theta}$ are the parameters that determines the network. In the process of resolving which hand-written digit is on a 28 by 28 pixel image, this function can be further clarified as the function $\mathbf{f}(\mathbf{x};\boldsymbol{\theta}) : \mathbb{R}^{784} \to \mathbb{R}^{10}$. The input is of dimension 784, as there are 784 input pixel values which range from 0 to 1, representing the greyscale with 0 for black pixels and 1 for white pixels. The output is of dimension 10 as there are 10 digits 0-9, with each output node displaying a number 0-1 depending on how certain the network is on which digit the image depicts. Furthermore, the parameters $\boldsymbol{\theta}$ are determined by the architecture of the network, described in the following section.

1.1.1.1 Architecture of a neural network

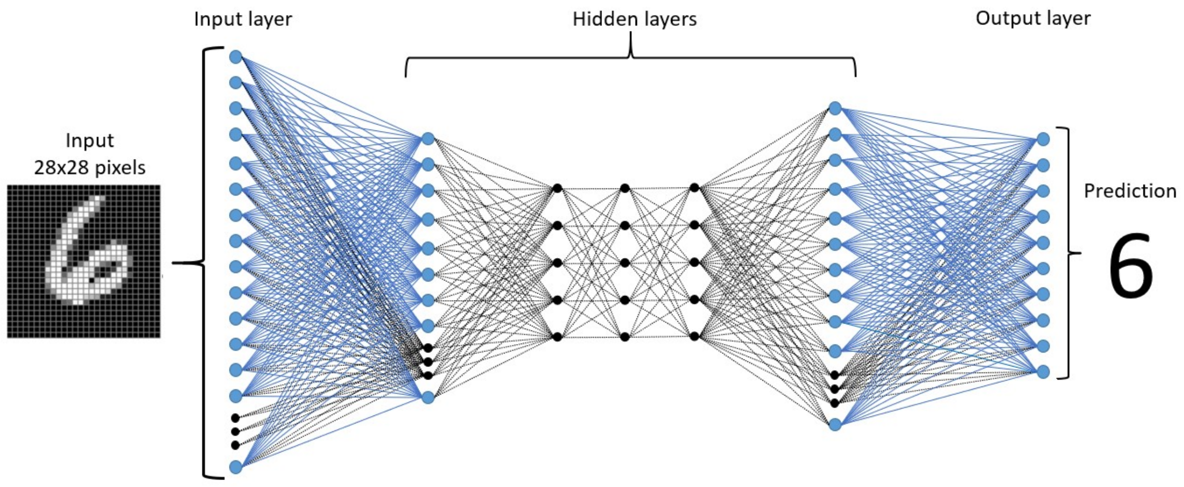


Figure 1: This figure illustrates how a basic neural network is built.

The basic architecture of a fully connected neural network is showcased in the figure above. The number of hidden layers and nodes in each of them is arbitrary, although an input layer with 784 nodes and an output layer of 10 nodes are required for this particular problem. A node in this case is simply a value, usually ranging from 0 to 1. This value is referred to as its *activation.*

The connection of one node to another node requires a *weight.* The weight determines how much the previous node's activation affects the current node's activation, mathematically described as $a^l = w^l \cdot a^{l-1}$, with the connection's weight as w^l, and activations given as a, with superscripts l and $l-1$ indicating which layer the nodes belong to. The weights need a starting value. A common initialisation of the weights, for a network with m inputs and n outputs using a uniform distribution U, is to use the Glorot initialisation, presented below. (Goodfellow et. al, 2016)

$$w \sim U\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right) \approx U\left(-0.087, 0.087\right) \tag{1}$$

Additionally, we might require a threshold, under which no activation is given at the current node. This is regulated using a *bias*, which using previous notation gives $a^l = w^l \cdot a^{l-1} + b^l$, where b^l is the current node's bias. It is not uncommon for networks to not have biases at all, although the one implemented in this problem has. Biases are usually initialised to zero. (Goodfellow et. al, 2016)

Lastly, the current node's activation needs to be controlled to land between 0 and 1 again, so we run this value through an *activation function*, which accomplished this. One common activation function is the sigmoid function, which is defined by

$$\sigma_{sigmoid}(z) = \frac{1}{1+e^{-z}}. \tag{2}$$

The sigmoid function gives a number close to 0 for small, or negative input z, and a value close to 1 for large z. Another common choice for an activation function is the rectified linear unit function (ReLu). This is defined as

$$\sigma_{ReLu}(z) = max(0, z). \tag{3}$$

The ReLu function cannot give negative values but can give infinitely large positive values, so the output range is not 0-1 as it is for the sigmoid function. This may seem problematic, but in practice, it works fine as the output is still compared with the correct value, which is within the range 0-1. In modern neural networks, the default recommendation is to use ReLu (Goodfellow et. al, 2016, p.171). ReLu is more computationally efficient as it just needs to pick $max(0, z)$, compared to the exponential operations for sigmoid. Additionally, the gradient of the sigmoid function vanishes for very small or large input, which is not the case for ReLu as it is either 0 or 1. The advantage of the sigmoid function is, as previously mentioned, that activation is limited between 0 and 1, and the risk of blowing up activation is avoided.

All activations in a layer can easily be written using matrix notation, with the current layer's activations as $\mathbf{a}^l$, the previous layer's activations as $\mathbf{a}^{l-1}$, all the weights of the connections between the nodes in each layers as $\mathbf{w}^l$ and all the biases at the current layer as $\mathbf{b}^l$, as

$$\mathbf{a}^l = \sigma(\mathbf{w}^l \cdot \mathbf{a}^{l-1} + \mathbf{b}^l). \tag{4}$$

Each node, except for the input nodes, is associated with an individual bias, and each connection with a weight. Collectively, all the weights and biases of a network form the parameters $\boldsymbol{\theta}$ referenced earlier. The dimension of $\boldsymbol{\theta}$ can easily grow very large, as showcased in a few examples below.

If the NN used in the current task of image classification and the NN had no hidden layers, but just an input layer of 784 nodes and an output layer of 10 nodes, this would give $784 \cdot 10 = 7840$ weights and 10 biases, and the dimension of $\boldsymbol{\theta}$ would be **7850**. If one hidden layer of 32 neurons are added between them, this would give $784 \cdot 32 + 32 \cdot 10 = 25408$ weights and $32 + 10 = 42$ biases, giving the dimension of $\boldsymbol{\theta}$ as **25450**. If a NN with 2 hidden layers of 400 neurons are used this gives $784 \cdot 400 + 400 \cdot 400 + 400 \cdot 10 = 477600$ weights and $400 + 400 + 10 = 810$ biases, giving $\boldsymbol{\theta}$ a dimension of **478410**. You easily see how the number of parameters grows rapidly with larger networks. This plays a large part in the computational demands of training a NN, as can be seen in the following section which describes this.

1.1.1.2 Training

The goal of this NN is to predict which digit is written on a given image. To accomplish this, the NN needs training. The process of training a NN is the central problem in both implementation and optimisation of a NN. By training the network, we mean the process of fitting all the weights and biases (gathered in $\boldsymbol{\theta}$) of the network to a given set of data. As most of the parameters (weights) in $\boldsymbol{\theta}$ are initialised randomly according to the Glorot initialisation ([1]), an untrained NN will give random results when an image is put through the system. Now, training is done by putting training images through the network and comparing the output with the desired results, which is possible as each image is labelled with its supposed digit. If the result is close to the desired result only small tweaks are made to the network, and vice versa if the result is far from the desired result. The comparison is done through a *cost function*, also called a *loss function*. One such cost function is mean square error (MSE). With the last layer's activations in $\mathbf{a}^L$ (output of the network) and their desired values in $\mathbf{y}$, the cost C using MSE in this problem is calculated through

$$C = \frac{1}{N} \sum_{i=1}^{N} ||\mathbf{a}_i^L - \mathbf{y}_i||^2. \tag{5}$$

Here, N is the number of images in the training dataset, which will be 60000 for this particular problem. The desired values $\mathbf{y}$ will be 0 for all nodes except for the correct one, which will be 1. The values in $\mathbf{a}^L$ between 0 and 1 describes how likely the network thinks the given image is any of the numbers 0-9. The problem of training the network now becomes a minimisation problem of the cost C. If C is thought of as a function $C\left(\mathbf{f}(\mathbf{x}; \boldsymbol{\theta}), \mathbf{y}\right)$, as $\mathbf{a}^L = \mathbf{f}(\mathbf{x}; \boldsymbol{\theta})$, the problem of minimising C with respect to parameters $\boldsymbol{\theta}$ can be accomplished through *gradient descent*. The idea of gradient descent is that the gradient of the function C with respect to parameters $\boldsymbol{\theta}$ gives the direction of the steepest increase of the function C. This gives the direction of the steepest decrease as the negative of the gradient. Iterating this process through all data means that one step in the training process is calculated through

$$\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} - \epsilon \cdot \nabla_\theta \left(C \left(\mathbf{f}(\mathbf{x}_t; \boldsymbol{\theta}_{t-1}), \mathbf{y}_t \right) \right). \tag{6}$$

Here, ϵ denotes the learning rate, or step size of the training process. This parameter is also the main focus of this report, and will be investigated in much further detail further on. Arrays $\mathbf{x}_t$ and $\mathbf{y}_t$ denotes the current image's pixel values as well as its label. If this process is completed for all training images, we should after some iterations theoretically reach some minimum value of the cost function. Computing the gradient of C for 60000 training images, will not prove effortless. Also remember that the dimension of $\boldsymbol{\theta}$ is often very large. A lot of optimisation strategies must be deployed to make this problem computationally achievable, the most common of which is *stochastic gradient descent*, described in the following section. (Goodfellow et. al, 2016)

The goal of training is obviously for the network to be able to perform well on previously unseen data, we call this the testing dataset. When a network becomes 'too' well-trained over the training dataset, to the detriment of testing performance is when *overfitting* occurs. A way to illustrate overfitting is by studying the gap between testing and training error, which becomes very large when the network is overfitted. The opposite of overfitting is *underfitting*, which is simply when the network is not well-trained enough. This theory explains why a network cannot simply keep training over the same training dataset to improve real-world performance. (Goodfellow et. al, 2016)

1.1.2 Stochastic gradient descent

Stochastic gradient descent (SGD) is the most commonly used optimisation algorithm in deep learning today. Using SGD is a way of making a compromise between accuracy and speed when it comes to calculating the gradient of the cost function at a specific location. (Goodfellow et. al, 2016)

In theory, it is possible to calculate the exact value of the gradient. Recalling from the previous section, it is very costly to perform this type of calculation as datasets and networks are usually very large. This approach leads to a very 'cautious' training algorithm, taking slow and steady steps in exactly the right direction before eventually finding a minimum of the function. (Goodfellow et. al, 2016)

The opposite philosophy by which to find the minimum would be to, instead of using the whole dataset to compute the exact gradient at every step, only use a single datapoint to execute a very rough approximation of the gradient at this location. This approach makes for a fast but inaccurate algorithm. One could hope that as more and more steps are taken, the algorithm converges to a minimum even though the steps individually are not presentable as the correct direction of the gradient. In summary, this leads to a fast, but somewhat uneven stepping pattern to the minimum compared to the first described approach. (Higham et. al, 2019)

SGD is a blend of the two algorithms above. With SGD every gradient is calculated using a *mini-batch* of data. A mini-batch is a share of the data in the dataset used to give a good representation of the correct gradient, without having to use all the data in every step. This makes for a faster training session as less data has to be analysed. Simultaneously, the path towards the minimum is hopefully shorter and more accurate than if only one datapoint is used to determine the gradient. It is important to know that SGD is not perfect as the gradient computations are only approximations of the real gradient and therefore introduces some noise into our calculations. (Goodfellow et. al, 2016)

A mini-batch consists of several randomly chosen datapoints from the dataset. The mini-batch can be created with different philosophies. One is to build it up by first shuffling the original dataset and thereafter picking the m first datapoints to perform the gradient approximation before taking the first step towards the minimum. For the second step, a mini-batch consisting of datapoints $m+1$ to $2m$ is used, and so forth. Another course of action is to randomly select the m datapoints from the dataset into each mini-batch. This is analogue to drawing one card, m number of times from an ordered deck of cards. After each card has been drawn it is put back into the pile again. The most prone difference of the two then is the fact that first shuffling the dataset will only make use of a single datapoint once, whilst randomly picking from the 'deck' would make it possible for one datapoint to be present in several mini-batches, and some not present in any. It would also, though not very probable, be possible that the same datapoint is used several times in one mini-batch. (Goodfellow et. al, 2016)

1.1.2.1 Back propagation

When performing SGD, the gradient of the cost function with respect to biases and weights needs to be calculated. A common way to achieve this is by using the *back propagation algorithm.*

Wanting to find the gradient of the cost function, the partial derivatives of this function with respect to each w^l_{jk} and b^l_j in the network, has to be calculated. Here, l represents the layer in which the weight or bias is present. In the case of the bias, the j represent the node number in layer l. In the case of the weights, w connects node k in layer l with node j in layer $l+1$. (Higham et. al, 2019)

Recalling from section 1.1.1.2, the expression of the cost function in equation (5) gives us how the cost depends on the values of the nodes at the output layer. From equation (5) it is seen that the cost is only dependent on the weights and biases through the value of the output layer $\mathbf{a}^L$ (Higham et. al, 2019). Further, it is convenient to define a new variable z as the value of a node in layer l contributed by the previous layer as

$$\mathbf{z}^l = \mathbf{w}^l \cdot \mathbf{a}^{l-1} + \mathbf{b}^l. \tag{7}$$

Further the definition of a^l is recalled from equation (4), giving

$$\mathbf{a}^l = \sigma(\mathbf{z}^l) \tag{8}$$

with σ as the activation function. At last, the *node error* is defined as δ^l_j

$$\delta^l_j = \frac{\partial C}{\partial z^l_j} \tag{9}$$

to describe how sensitive the cost function is to a change in the value of z of node j at layer l. Finally, this yields the four equations of back propagation

$$\begin{aligned}
&\delta^L = \nabla_a C \odot \sigma'(z^L) \\
&\delta^l = (((w^{l+1})^T)\delta^{l+1}) \odot \sigma'(z^l) && \text{for} \quad 2 \leq l \leq L-1 \\
&\frac{\partial C}{\partial b^l_j} = \delta^l_j && \text{for} \quad 2 \leq l \leq L \\
&\frac{\partial C}{\partial w^l_{j,k}} = a^{l-1}_k \delta^l_j && \text{for} \quad 2 \leq l \leq L,
\end{aligned} \tag{10}$$

all derived from the chain rule. For the full derivation of the equations (10), see reference (Higham et. al, 2019). At last, the notation $\odot$ needs to be described. The sign denotes a *Hadamard product* which is an elementwise multiplication of two vectors of the same size. This means that in a Hadamard multiplication of vectors x and y $(x \odot y)$, the component i of the Hadamard product is calculated though $(x \odot y)_i = x_i \cdot y_i$. (Higham et.al, 2019)

1.1.2.2 Learning rate and stepping schedules

One of the most important parameters when setting up the training of a neural network is the learning rate ϵ. The learning rate is the parameter deciding the step size by which to go in the opposite direction of the gradient. The size of the learning rate is crucial, as a well-chosen learning rate will be hugely beneficial for the learning procedure. An ϵ too large will make the learning procedure very oscillative. On the other hand, a small ϵ makes the learning slow, though delivering a relatively smooth path towards the minimum.

An issue when dealing with SGD in tandem with a constant learning rate during a whole training session is the fact that SGD introduces noise in the gradient calculations. This is alright as long as the training algorithm is not close to a local minimum in the cost function. When closing in on a minimum, the noise in the gradient calculation will be large in proportion to the 'real' gradient, leading to taking random steps around the minimum. This phenomenon is often called a *noise ball*. It can be interpreted as how close SGD gets to a minimum, when the number of iterations in training goes to infinity, before the noise in the calculations takes over. The noise ball can be seen as a convergence size for SGD. The step size is simply too large to enable SGD to get any closer to a minimum, and 'bounces' around the minimum. The size of the noise ball is proportional to the learning rate ϵ. For accurate solutions, a small noise ball is ideal. There is however a trade-off, as a small learning rate increases convergence time. For the proof of noise ball, see reference (Cornell CS, 2017).

To counteract the noise ball, a variable learning rate could be helpful. The denotation of ϵ could now be changed to ϵ_k, where k ranges from 1 to n during n iterations of the training process. How ϵ_k changes during training is defined by a *stepping schedule* providing a good set of values for the learning rate. More on this later. (Goodfellow et. al, 2016)

In theory, not using SGD but the whole dataset, to calculate the gradient in each step would make a stepping schedule superfluous. This is because this method, though slow, will produce the exact value of the gradient at each location of parameter space. This means that close to a local minimum, the gradient will be small and at that minimum, the value of the gradient would be zero. (Goodfellow et. al, 2016)

There are a number of different stepping schedules providing more stability and reducing the impact of noise close to a minimum of the cost function. To begin with there are a number of set schedules depending on mathematical functions. Examples of these types of schedules are *exponential decay* (equation (11)), *inverse time decay* (equation (12)), *piecewise constant decay* (equation (13)) and *polynomial decay* (equation (14)) (TensorFlow, 2021). Below, the formulas of calculating the learning rate at step k can be seen.

$$\epsilon_k = \epsilon_0 \cdot \gamma^k \tag{11}$$

$$\epsilon_k = \frac{\epsilon_0}{1+\gamma^k} \tag{12}$$

$$\epsilon_k = (\epsilon_0 - \epsilon_n) \cdot (1 - \frac{k}{n}) + \epsilon_n \tag{13}$$

$$\epsilon_k = (\epsilon_0 - \epsilon_n) \cdot (1 - \frac{k}{n})^p + \epsilon_n \tag{14}$$

Above, ϵ_0 is the initial learning rate, ϵ_n is the end learning rate, γ is the *decay rate* which determines how fast the learning rate is to decrease, k is the present step in the training session, n is the total number of changes of the learning rate in the stepping schedule and p is a selectable coefficient.

As a part of implementing a stepping schedule, it is central to know when these learning rates should be updated. This can be done in several ways. One way could be to update the learning rate after each mini-batch and therefore after each taken step. Another philosophy could be to update the learning rate after each *epoch*, which is another term needing an explanation. An epoch is defined as when an entire training dataset has been passed through the neural network once in the training session (Sharma, 2017). Usually, the training session consists of several epochs, meaning the whole dataset will have been used to train the neural network several times in trying to get a sufficiently accurate network.

It can be shown that inverse time decay, given by (12), is an optimal stepping schedule for convex problems (Cornell CS, 2017). However, as neural network training is not ordinarily a convex optimisation problem, this stepping schedule might not be optimal for this particular problem.

1.1.2.3 Adaptive learning rate and ADAM

The stepping schedules presented in the sections above do not take into account what the surrounding of the cost function looks like or what step sizes and gradients have been used before. From an optimisation standpoint, it could be beneficial to choose ϵ_k based on these criteria and not only follow a fixed mathematical formula. Algorithms that do this are said to use an adaptive learning rate.

One of the most widely used adaptive learning rate algorithm today, which have shown to be effective in a lot of different deep learning implementations, is the *ADAM algorithm* (DeepLearningAI, 2017). ADAM in itself is a continuation and development of two other optimisation algorithms called *momentum* and *RMSprop* (Bushaev, 2018).

The basic idea behind momentum is to take into account not only the value of the gradient at the present location, but also let it be influenced by an exponentially decaying moving average of previous values of the gradient. In theory, this means speeding up learning in especially steep or ravine-shaped regions in parameter space. A momentum implementation could also conquer a small hill to later finding its way to a new 'better' minimum, contrary to a non-adaptive stepping schedule getting stuck in the first local minimum. (Goodfellow et.al, 2016)

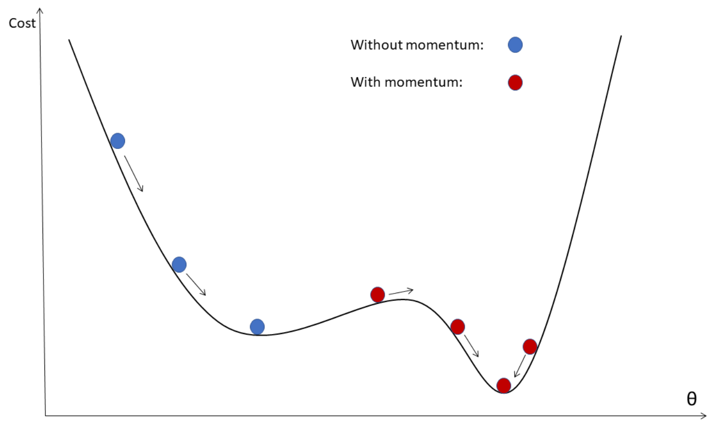


Figure 2: Shows difference in behaviour between momentum and non-momentum implementation.

The RMSprop algorithm calculates an appropriate step size in parameter space by scaling all the model parameters, weights and biases, 'inversely proportional to the square root of the sum of all the historical squared values of the gradient [and] changing the gradient accumulation into an exponentially weighted moving average'(Goodfellow et.al, 2016, p. 303). By doing this, RMSprop changes the learning rate as the training proceeds but only as much as the nearest history of surroundings suggest. This is favourable as the shape of parameter space can change during the path towards a minimum, requiring an ability to local adaptation in the learning rate. (Goodfellow et.al, 2016)

ADAM is, as mentioned, a combination of the two algorithms explained. The first step of the algorithm is to calculate the influence of momentum and RMSprop on the step size.

$$\begin{aligned} V_{dw_t} &= \beta_1 V_{dw_{t-1}} + (1-\beta_1) dw_t \\ S_{dw_t} &= \beta_2 S_{dw_{t-1}} + (1-\beta_2) dw_t^2 \\ V_{db_t} &= \beta_1 V_{db_{t-1}} + (1-\beta_1) db_t \\ S_{db_t} &= \beta_2 S_{db_{t-1}} + (1-\beta_2) db_t^2 \end{aligned} \tag{15}$$

Equation (15) shows formulas to calculate the following: V_{dw_t} and V_{db_t} which are the momentum exponentially weighted average at step t for weights and biases. S_{dw_t} and S_{db_t} which are the RMSprop exponentially weighted average at step t for weights and biases. In equation (15) dw and db are the gradient of the cost function with respect to weights and biases calculated with back propagation at step t. β_1 and β_2 are two hyperparameters commonly set to $\beta_1 = 0.9$ and $\beta_2 = 0.999$. At the start of the training the values of V_{dw_t}, S_{dw_t}, V_{db_t} and S_{db_t} are set to be 0. (DeepLeraningAI, 2017)

It is necessary to correct the calculated parameters in equation (15) from a certain degree of bias. How this is done is shown in equation (16). (DeepLearningAI, 2017)

$$\begin{aligned} \hat{V}_{dw_t} &= \frac{V_{dw_t}}{1-\beta_1^t} \\ \hat{S}_{dw_t} &= \frac{S_{dw_t}}{1-\beta_2^t} \\ \hat{V}_{db_t} &= \frac{V_{db_t}}{1-\beta_1^t} \\ \hat{S}_{db_t} &= \frac{S_{db_t}}{1-\beta_2^t} \end{aligned} \tag{16}$$

Finally, the update of the weights and biases are as follows in equation (17).

$$\begin{aligned} w_t &= w_{t-1} - \alpha \frac{\hat{V}_{dw_t}}{\sqrt{\hat{S}_{dw_t}} + \lambda} \\ b_t &= b_{t-1} - \alpha \frac{\hat{V}_{db_t}}{\sqrt{\hat{S}_{db_t}} + \lambda} \end{aligned} \tag{17}$$

Here, α is a parameter that has to be tuned for the specific neural network and problem. λ is a parameter to avoid division by zero, set to 10^{-8}.

1.1.3 TensorFlow, Keras and MNIST

TensorFlow is an end-to-end open-source platform for machine learning by Google. Specifically, an interface within TensorFlow, Keras is used in this project. Keras is a deep learning API for Python, with a library of functions for building, training and testing NN:s. However, as this project aims to implement the entire neural network from scratch, the use of this library is very limited within this project, although it is a good way to get started with neural networks. Within Keras, there are multiple datasets built-in, which can be used for training the network. For this project, mainly the MNIST dataset was used, MNIST for 'Modified National Institute of Standards and Technology'. The MNIST dataset consists of 70000 images of hand-written digits, 28 by 28 pixels in size, all labelled with what images these are supposed to be. Of the 70000 images, 60000 are reserved for training the network and 10000 for validation and testing. Examples from the dataset are shown in Figure 3. (TensorFlow, 2021)

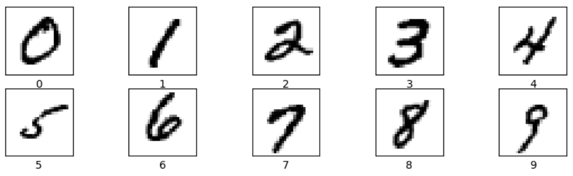


Figure 3: MNIST

1.2 Issue

Issues being dealt with in this report are the following:

- Does a stepping schedule improve the performance of the training of a neural network?
- Will a stepping schedule improve the classification of data made by the neural network?
- If a stepping schedule proves to be beneficial to use, does it hold for all circumstances?
- How do stepping schedules hold up to adaptive optimisation methods, such as ADAM?

1.3 Delimitations

When investigating the effect of using a stepping schedule while training a neural network, a few delimitations have been made. The delimitations are presented below:

- Only fully connected neural networks have been studied.
- Only three different sizes of neural networks have been analysed, with 2 hidden layers maximum.
- Only five traditional stepping schedules and one adaptive optimisation algorithm have been tested.
- Only one dataset have been used.

2 Methodology

Here follows an explanation of the methodology used in this project.

2.1 Literature

The field of neural networks contains many concepts, as you probably realised from the background section. A good piece of literature covering all of the basics is *Deep learning* by Goodfellow et. al. This book became the main reference for the first part of our literature study, offering insight into all basic and higher-level aspects of a neural network. Following the first part of the study, which focused on theoretical aspects of neural networks and learning, a deeper understanding of practical forms was required. For this part, the report *Deep Learning: An Introduction for Applied Mathematicians* by Higham et. al, became a large part of the study. As this report repeats many of the concepts presented by Goodfellow et. al, but also implements them as examples in *MATLAB*, the gap between theory and practice was reduced.

2.2 Implementation

The goal of the implementation is to build, train and evaluate a neural network from scratch in Python, without using libraries such as Keras in TensorFlow. Bearing this in mind, the work began with a simple implementation of a NN in Keras. This enabled us to adjust settings such as layers, nodes, activations, stepping schedules and such in order to obtain an understanding of how each setting affects the performance of a neural network, without actually understanding the code. This played a vital role in building an understanding of a NN, and preparing for writing a NN from scratch in Python.

The process of implementing the NN from the ground up was, to begin with, very straightforward. The implementation had a focus on modularity, meaning all parameters should be modifiable by the user without issue. A NN needs layers, with weights and biases connecting each node in one layer to every node in the next layer. They need an activation function as well as a cost function. The NN needs parameters such as number of layers and their sizes, initialisations of weights and biases. All the weights of a layer are implemented as a matrix where rows and columns correspond to the previous and the current layers respectively. The biases of the layers are implemented as an array with one value per node in the current layer. The weight-matrices and bias-arrays for all layers are kept in basic NumPy Python-lists. Now, the activation of one layer can be calculated using equation (4). The activation function used is ReLu, seen in equation (3). With all this in place, the architecture of the NN is finished. The challenge becomes training the network.

The process of training the network relies heavily on the mathematical conclusions presented in the background section, namely the equations of back propagation (10). The implementation of back-propagation was assisted by the examples in MATLAB presented by Higham et. al, and finally yielded a function that calculated the gradient of the cost function with respect to all the weights and biases for a mini-batch. The algorithm then takes a step in the opposite direction of the gradient for all parameters, in accordance with the process of stochastic gradient descent. SGD is thoroughly presented in the background section 1.1.2.

Next, the training process was divided into sections, with each running a certain number of mini-batches. Using SGD means that not all the 60000 images must be treated, since images are selected randomly from the dataset. This sped up the training process significantly. The default choice was to evaluate 10% of the data (6000 images) in each section in mini-batches of 16, giving 375 mini-batches per section. Typically, 10 sections were run, giving the total number of images treated as 60000, and the total number of batches as 3750. Further, implementing stepping schedules means that after each section, the learning rate is decreased according to the given schedule.

To compare schedules, two parameters were studied; training loss and testing accuracy. These were evaluated after each batch. Training loss was calculated using MSE in accordance with equation (5) for all images in the batch. Testing accuracy was calculated using 50 random images from the testing dataset. The fraction of these correctly predicted gave the training accuracy. Using all the 60000 training images in batches of 16 in training, which gives $60000/16 = 3750$ batches and as many data-points for training loss and testing accuracy. Please refer to the code found in `https://github.com/axeboii/Neural-Network` if you are curious about the implementation.

2.3 Optimisation and visualisation

When investigating the stepping schedules' effect on the loss function and accuracy, a trial and error philosophy was used. The parameters, such as learning rate and decay rate, was tuned until satisfactory properties of the network was obtained. The optimal parameter for every stepping schedule was noted and used in the evaluation of the schedules. Also, worse than optimal parameters were chosen and noted for each stepping schedule to make it possible to present the impact of the parameters in plots.

When collecting data for visualisation, ten separate learning sessions were performed to make the results more trustworthy and less dependent on randomness. The datapoints collected were processed so that the mean of the ten training sessions was gained. To make the results more readable the number of datapoints was reduced from the number of steps taken, 3750, to 50. This was made by averaging every 75 steps to generate one single datapoint from that information. This reduced the noisy nature of the original data. The results were presented in plots. This approach to visualisation was used independently of the test performed and shown.

2.4 Parameter settings

The parameters used, if nothing else is noted, is seen below.

Table 1: The parameters used with the different schedules.

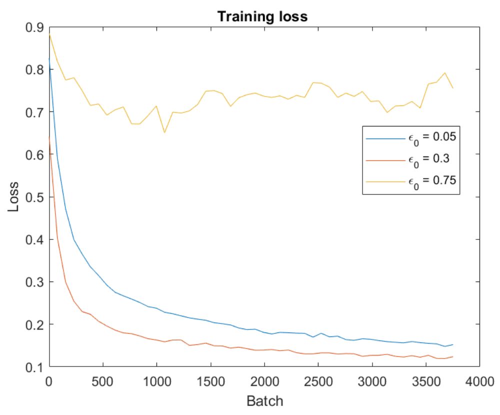
Stepping schedule	**Inital learning rate ϵ_0**	**Decay rate γ**	**End learning rate**
No schedule	0.3	-	-
Piece wise constant decay	0.3	linear	0.055
Exponential decay	0.5	0.75	-
Inverse time decay	0.5	0.5	-
Polynomial decay	0.3	2.5	0.01

With ADAM, the parameters used were $\alpha = 0.003$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\lambda = 10^{-8}$.

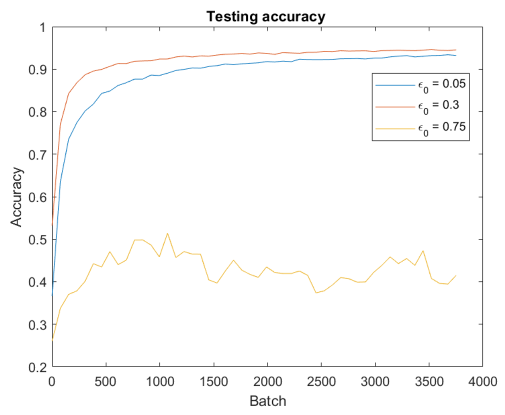
3 Result

3.1 Training with constant learning rate

Figure 4 showcases how learning rate affects the training process. Figure 4a shows the loss of each batch, and Figure 4b shows the accuracy when testing the network with test-images after each batch. No stepping schedule is used. The network has one hidden layer with 32 nodes.



(a) Training loss.

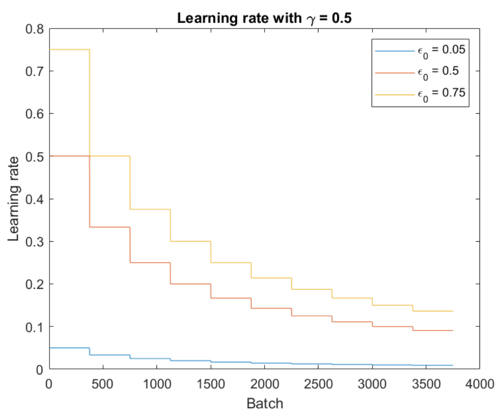


(b) Testing accuracy.

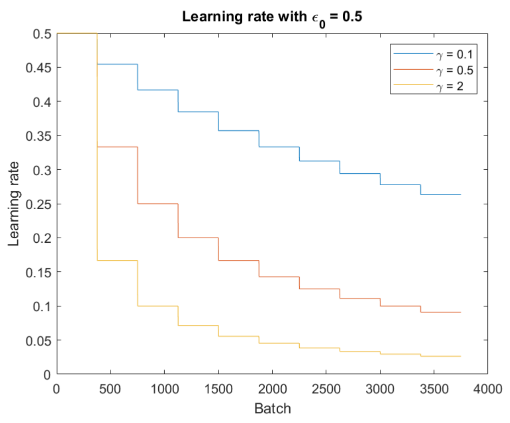
Figure 4: These figures show how loss and accuracy are affected by the learning rate ϵ in the case of no stepping schedule.

3.2 Training with stepping schedules

Next, the inverse time decay schedule is studied. Varying the parameters ϵ_0 and γ the following learning rates are used.



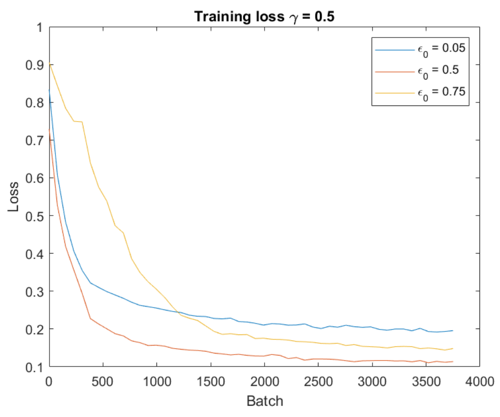
(a) Learning rate with varying initial learning rate ϵ_0.



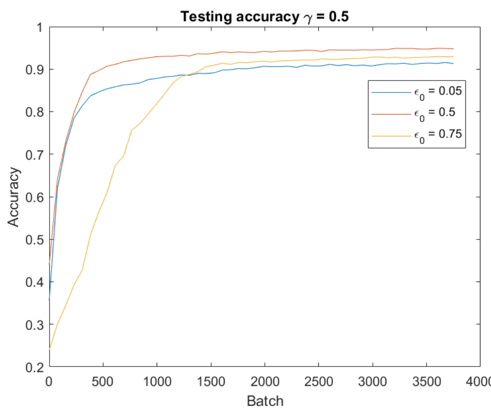
(b) Learning rate with varying decay rate γ.

Figure 5: These figures show how the learning rate is affected parameters ϵ_0 and γ for the inverse time decay schedule.

Now, these learning rates are implemented and gives Figure 6 and 7, which shows loss and accuracy corresponding to a change in initial learning rate with either a constant decay rate of $\gamma = 0.5$, or constant initial learning rate $\epsilon_0 = 0.5$.

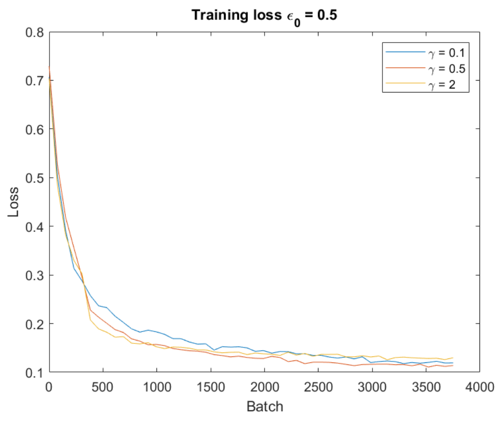


(a) Training loss.

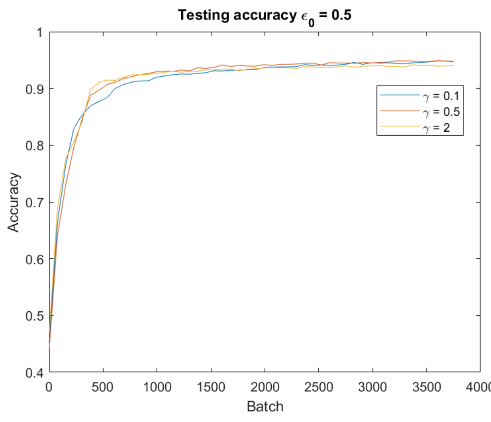


(b) Testing accuracy.

Figure 6: These figures show how loss and accuracy are affected by initial learning rate ϵ_0 for the inverse time decay schedule. Decay rate γ is kept constant.



(a) Training loss.



(b) Testing accuracy.

Figure 7: These figures show how loss and accuracy are affected by decay rates γ for the inverse time decay schedule. Initial learning rate ϵ_0 is kept constant.

The other stepping schedules are now studied. Figure 8 shows how the learning rate varies during a training session for settings found in Table 1, whilst Figure 9 shows how loss and accuracy are affected.

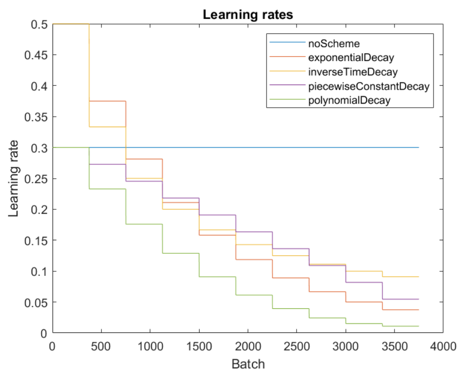
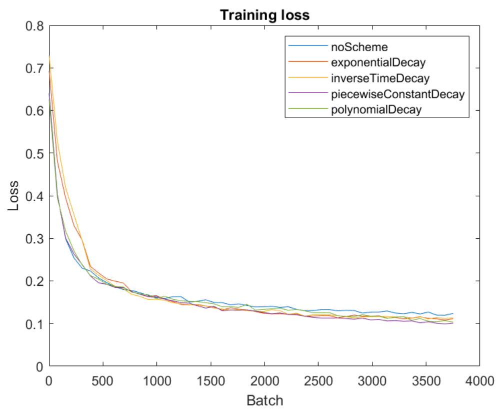
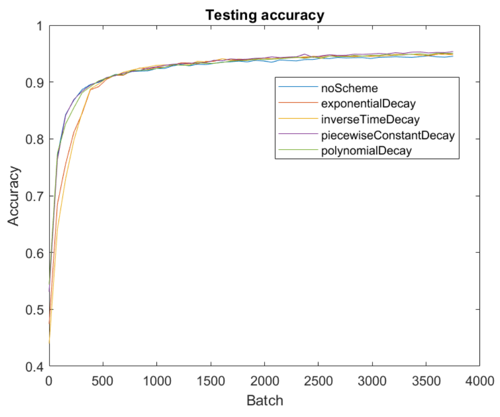


Figure 8: This plot shows how the learning rate varied in the different schedules.



(a) Training loss.

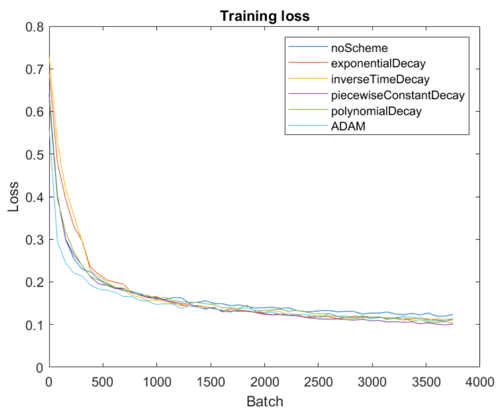


(b) Testing accuracy.

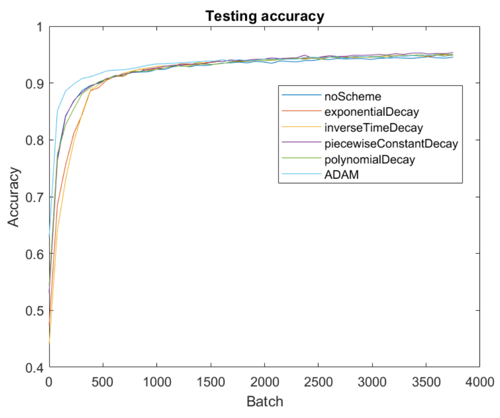
Figure 9: These figures show how loss and accuracy are affected by different stepping schedules.

3.3 Training with adaptive learning rate

ADAM is now compared to the regular stepping schedules. Figure 10 shows the performance.



(a) Training loss.

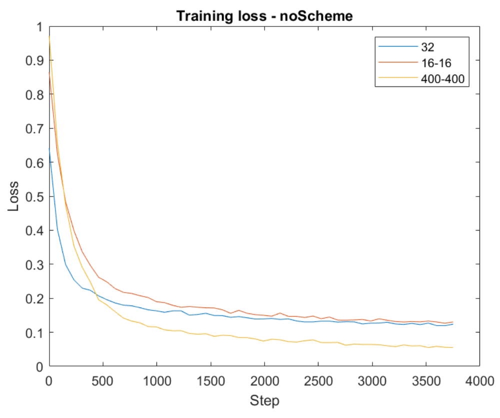


(b) Testing accuracy.

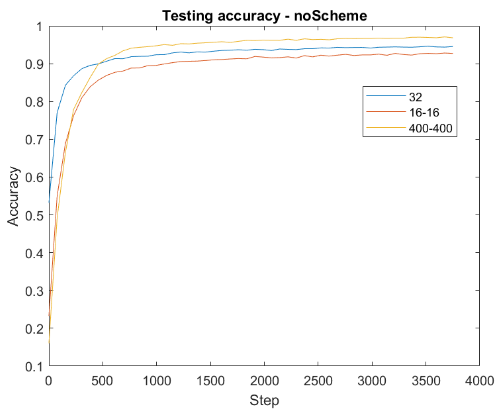
Figure 10: These figures show how loss and accuracy are affected by ADAM with respect to the other stepping schedules.

3.4 Network size

It is interesting to study how the results might be impacted by network structures and sizes. Figure 11 shows loss and accuracy when using a constant learning rate $\epsilon = 0.3$ for three different sizes of the hidden layers. From now on '32' indicates that a network of one hidden layer with 32 nodes has been used. The notation '16-16' and '400-400' indicates that two hidden layers have been used with 16 and 400 nodes in each layer respectively.



(a) Training loss.

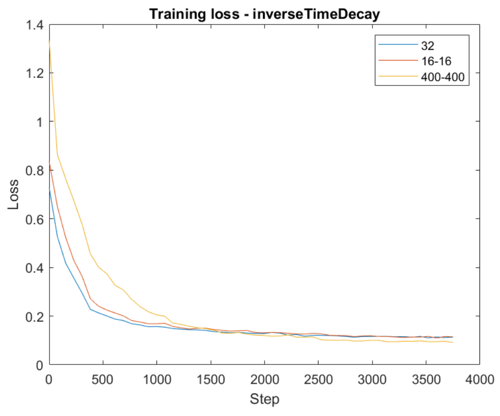


(b) Testing accuracy.

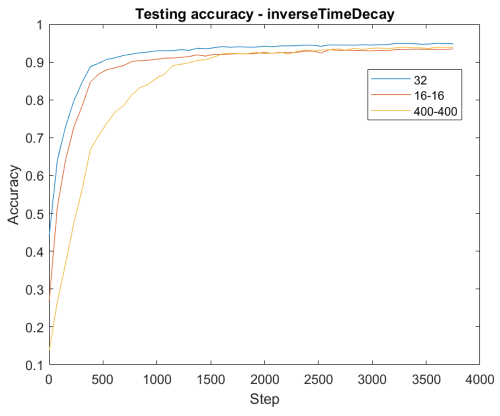
Figure 11: These figures show loss and accuracy with no stepping scheme and hidden layers of different sizes with $\epsilon = 0.3$.

As the slope of the yellow 400-400 curve is so steeply declining throughout training, a test with longer training was implemented. It ran for 187500 batches, 50 times the current amount. A result of testing accuracy over 98% was achieved, although severe overfitting was observed as training loss reached almost 0.

Implementing a stepping schedule (the inverse time decay schedule) for the different sizes gives Figure 12, which shows loss and accuracy with the three network sizes. Parameters from Table 1 are used.



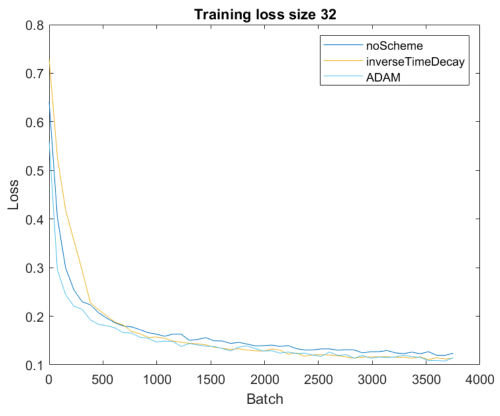
(a) Training loss



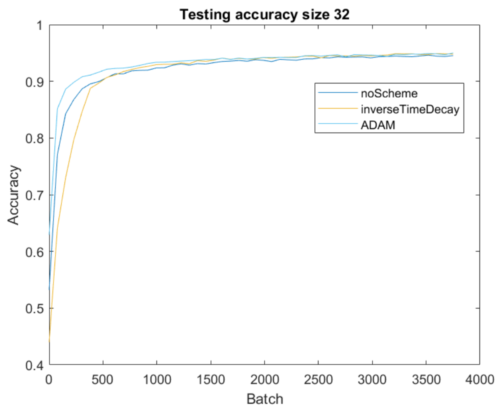
(b) Testing accuracy.

Figure 12: These figures show loss and accuracy with inverse time decay using $\epsilon = 0.5$, $\gamma = 0.5$ and hidden layers of different size.

In order to study how stepping schedules are affected by network sizes, no scheme, inverse time decay and ADAM are plotted together for the different network sizes. This gives Figures 13, 14 and 15. Parameters from Table 1 have been used.

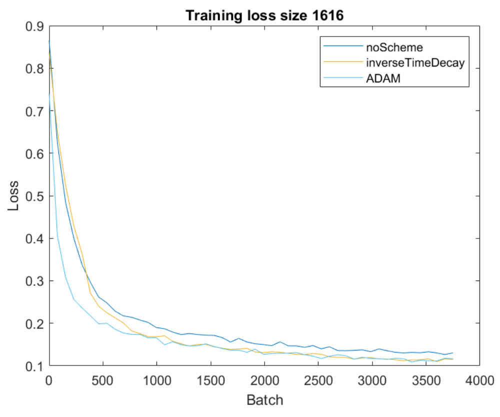


(a) Training loss

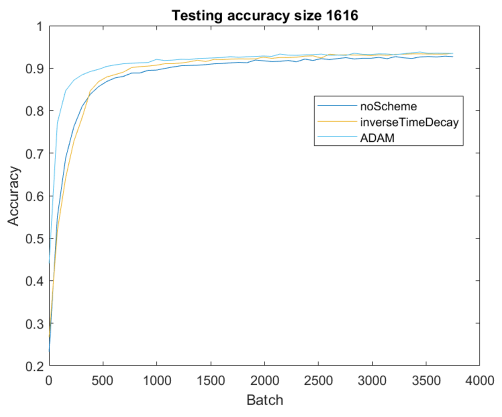


(b) Testing accuracy

Figure 13: Loss and accuracy for a hidden layer of size 32 with respect to different stepping schedules.

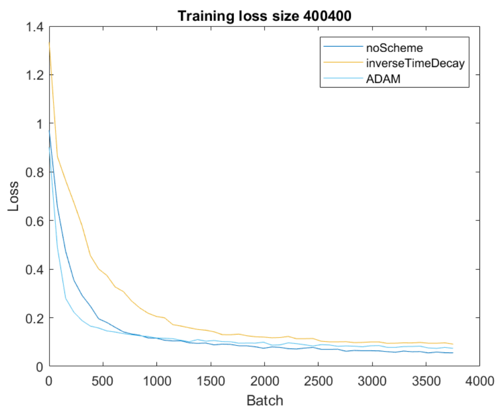


(a) Training loss

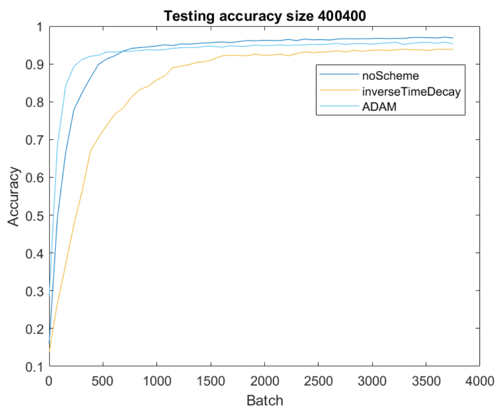


(b) Testing accuracy

Figure 14: Loss and accuracy for hidden layers of sizes 16-16 with respect to different stepping schedules.



(a) Training loss



(b) Testing accuracy

Figure 15: Loss and accuracy for hidden layers of sizes 400-400 with respect to different stepping schedules.

3.5 Code

The written code containing the full implementation is found in the following GitHub repository. All generated data (loss and accuracy values) are also found here as .dat files, named with the particular parameters studied and settings used `https://github.com/axeboii/Neural-Network`.

4 Analysis

4.1 How learning rate affects learning

Studying the results from Figure 4, it is clear how the training of a network is dependent on the size of the learning rate. With a constant learning rate throughout training, the setting $\epsilon = 0.3$ proved to perform the best. A lower setting, $\epsilon = 0.05$, gives slower learning and would probably reach the level of the higher setting after some more training. A higher setting such as $\epsilon = 0.75$ proved to not give much learning at all, as SGD is observed to converge into a large noise ball. These results are in line with what we would expect from theory, and a valuable lesson has been learnt as to which learning rate works best for this problem.

4.2 How stepping schedules affects learning

Optimising the settings for the inverse time decay schedule, we see how the initial learning rate ϵ_0 and decay rate γ affects the learning process. Figure 6 show that a high initial learning rate, $\epsilon_0 = 0.75$, gives slow learning as it converges to a large noise ball when learning rate is high. Clear jumps can be seen when the learning rate is lowered according to the schedule. A lower initial learning rate, $\epsilon_0 = 0.05$, gives fast learning in the beginning, but soon becomes slow and never reaches high accuracy. Figure 7 shows that the decay rate γ does not seem to have as large of an impact on learning as ϵ_0. This is surprising, as the variation in learning rate is quite drastic, which can be seen in Figure 5b. This may be explained by the fact that the learning rate is the same for the first 375 batches before the first step in the schedule is taken. This means that the minimum has been approached sufficiently for the higher decay rates to still yield effective learning.

Regarding the three other stepping schedules, it is from Figure 9 not obvious to see how they affect learning. The difference between them is small, as can be seen from Figure 8. Unsurprisingly, this leads to very similar loss function values and testing accuracy between the four schedules. However, since they all are very different to a constant learning rate, it is not far fetched to expect the training process to also differ significantly. It turns out that all the schedules perform slightly better than no stepping scheme in the end and slightly worse at the beginning of training. For the default network, polynomial decay gave the best result in the end, although the margins are very small to other schedules. Furthermore, the optimal stepping schedule for convex problems, inverse time decay, was not observed to be optimal for this particular problem. This is not unexpected, as the training of a neural network is not generally a convex problem.

We can conclude that the largest contributing factor to an effective training algorithm is a well-chosen initial learning rate, rather than choosing the right stepping schedule. For this problem, a stepping schedule might not even be worth implementing as the benefits are so marginal to using a constant learning rate.

4.3 How adaptive schedules affects learning

As described in section 1.1.2.3, the adaptive stepping schedule ADAM has a few unique properties that hopefully would improve the learning of a neural network. As can be seen in Figure 10 the ADAM algorithm seems to accomplish similar testing accuracies as the more traditional stepping schedules. However, ADAM seems to be beneficial to the speed of the improvement of the network parameters, shown by the steeper slope at the beginning of the graph in Figure 10b. The speed of the way the accuracy improves with ADAM may be due to a very well adapted step size to the surrounding parameter space. The ADAM algorithm is probably able to adapt better than a simpler predetermined stepping schedule in this case. In theory, ADAM should have the opportunity to perform better also further into the training session. Why this is not true for this case, as can be seen in Figure 10b, is still unclear.

Peeking into the next section, where different networks are implemented, and analysing Figures 13, 14 and 15 the same trends as above can be observed. The ADAM algorithm seems to have an advantage in the early stages of the training with the other stepping schedules managing to equal or better ADAM's result in the end.

4.4 How network size affects learning

Looking at the results presented in section 3.4, some interesting points can be made. At the larger network size, with two hidden layers of 400 nodes, no stepping schedule performed significantly better than with the default hidden layer of 32 nodes as can be seen in Figure 11. At the same time, the smaller network with two hidden layers of 16 nodes performed worse. Seemingly, more parameters give a better performing network. On the contrary, the behaviour is completely different when training with a stepping schedule (inverse time decay, the optimal stepping schedule for convex problems). Here, the larger network of 400-400 nodes performs worse in the beginning, and basically on par at the end of training. The same is true for the smaller network of 16-16 nodes, although it is faster at the beginning of training. The network with one layer of 32 nodes performs best. We do also see some overfitting tendencies for the 400-400 and 16-16 node networks, as their training loss is better than the 32-network whilst having a worse testing accuracy.

Comparing optimisation schedules for the three network sizes it can be seen that inverse time decay is the slowest for all sizes, but recovers and performs on par with ADAM at least for smaller networks. For the smaller networks, no stepping scheme performs averagely in the beginning and worst in the end. For the larger network, however, no schedule clearly performs the best, although ADAM is faster in the beginning.

4.5 Sources of error

As the implementation of a neural network in Python is quite extensive, it is of course possible that small errors can be present in the code. However, as testing accuracy over 98% was achieved it is reasonable to assume that no large errors are present in the network's implementation. The high accuracies need discussion, as they might pose a problem in the comparison between optimisation methods and hence the conclusion in this report. The issue of classifying handwritten digits from the MNIST dataset is commonly thought of as an easy task for a neural network, proven by our results where testing accuracies of 94-95% was easily reached. With accuracies this high, differences between stepping schedules and constant learning rates might be slightly concealed, possibly hindering us from reaching certain conclusions. If the same study were to be performed on a more difficult classification problem, such as Fashion MNIST, we might have reached a clearer result.

Another source of error also concerns the drawn conclusion. It is possible that not enough different networks and stepping schedules were tested, which leads to the conclusion of whether or not stepping schedules helps optimise training possibly not being applicable for all networks. All networks implemented and tested in this project are relatively shallow. It is possible that stepping schedules would make a more significant difference if deeper networks were to be tested.

5 Conclusion

Summing up the results it is clear that a stepping schedule does not improve learning independently of other parameters. Generally speaking, the ADAM algorithm seems to speed up learning initially but as this speed trails off, it is unclear if that is significant in an applied situation. Looking at the other stepping schedules, they seem to perform better than using a constant learning rate in certain situations, but worse in others.

It is important to know the delimitations of this report as it is only concluded for the tested circumstances that a stepping schedule does not seem to improve learning significantly. Further testing is required to know whether stepping schedules are beneficial in the general case or not. In further research, it would be interesting to investigate the stepping schedules' impact when using other data sets together with different depths and widths of networks. Also other parameters such as batch size and how often the learning rates are updated could be interesting parameters to tweak. Different and more difficult classification problems would also be interesting to investigate further.

Lastly we could bring up some of the ethical aspects of the issues brought up in this report and to machine learning as a whole. Of course, the fast development in machine learning makes for quite a few ethical questions needing to be addressed. As seen in China, governments can use machine learning and AI to control and monitor their citizens in a way they deem suitable. This is a violation of the human right of freedom. On the other hand, AI and machine learning could be very helpful in our everyday life when used in non-surveillance and non-war situations, such as medical implementations, autonomous cars and industrial automation. As the algorithms behind AI becomes more effective and better optimised, we can't help wondering about whether or not improving AI is improving the world we live in. We hope that AI will improve the world, and not be misused. Education is a necessary first step, and something we hope this report is contributing towards.

Acknowlegdements

We direct a great thank you to Anna Persson, our supervisor, who helped us with finding relevant literature and discussing ideas and results throughout this project. We would also like to thank Anton Sederlin who helped us setting up a GitHub repository for the code in this project.

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7 Appendix

7.1 Word list

Activation function - The function σ used to control the activation of a node, see equation (4).

ADAM - An optimisation algorithm that uses an adaptive learning rate, see section 1.1.2.3.

Back propagation - The method used for updating weights and biases of a network in training, see section 1.1.2.1.

Bias - A node parameter b, used to calculate the activation of a node, see equation (4).

Cost function - A function to calculate the distance from the prediction and the optimum value of an image. In this project, mean squared error is used, see equation (5).

Dataset - A cluster of data. In this case, the MNIST dataset is used.

Decay rate - A parameter used in certain stepping schedules to determine how fast the learning rate is decreased.

Keras - A deep learning API for python within TensorFlow, with a library of functions for building, training and testing neural networks.

Layers - Layers consist of nodes and are what builds the network. Divided into an input layer, hidden layers and an output layer.

Learning rate - A parameter that determines how large steps are taken in learning.

Loss function - Same as cost function.

Mini-batch - A group of randomly selected datapoints used to calculate a gradient.

MNIST - A dataset containing 70000 labelled images of handwritten digits.

Noise ball - A convergence size for SGD.

Overfitting - Overfitting occurs when a network becomes too optimised for a training dataset, to the detriment of performance for new data.

ReLu - A common activation function, see equation (3).

Sigmoid function - A common activation function, see equation (2).

Stepping schedules - Predetermined schemes of how to decrease learning rate during training, see section 1.1.2.2.

Stochastic gradient descent (SGD) - A common method in neural network training that utilises mini-batches of datapoints instead of the entire dataset.

TensorFlow - An end-to-end open-source platform for machine learning by Google.

Weight - A node parameter w, used to calculate the activation of a node, see equation (4).