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Implementing neural networks in Accelerate

by

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Abstract

GPU-accelerated programming is used to speed up neural network computations. However, the main languages for GPU programming are CUDA and OpenCL, which are very low-level languages. This thesis proposes implementing a simple feed-forward back-propagation neural network, namely a convolutional neural network using Accelerate. Accelerate is an Embedded Domain-Specific Language in Haskell for GPU programming and has several accessibility advantages over CUDA, while still offering competitive performance. Once the implementation is successful, I plan to assess its performance, benefits and disadvantages against the traditional approaches with CUDA.

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I am very grateful to have learned so much during Thesis A, and look forward increasing my knowledge further in Thesis B!

Abbreviations

BGD Batch gradient descent learning algorithm

ConvNet Convolutional neural network

CUDA Computer Unified Device Architecture

DNN Deep neural network

EDSL Embedded domain-specific language

FFBP Feed-forward back-propagation algorithm

GPU Graphics Processing Unit

OpenCL Open Computing Language

PLS UNSW Programming Languages and Systems group

ReLU Rectified Linear Unit activation function

SGD Stochastic gradient descent learning algorithm

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Chapter 1

Introduction

Neural networks are widely used for computer vision and one of the best methods for most pattern recognition problems [NVI14]. For instance, Deep neural networks (DNN) can already perform at human level on tasks such as handwritten character recognition (including Chinese), various automotive problems and mitosis detection.

One issue with DNN is its compute-intensiveness. Training a neural network with massive numbers of features require a lot of computations. Unfortunately, the most efficient and economical approach to testing the validity of many hypotheses is repeated trial-and-error [Ng16].

For the above reason, neural networks implemented with GPU-accelerated computing are common, as such arrangements are generally faster than with a CPU cluster. The main languages for GPU programming are Compute Unified Device Architecture (CUDA) or Open Computing Language (OpenCL). Both are very low-level languages based on C/C++.

On the other hand, Accelerate is a embedded domain-specific language (EDSL) created for GPU programming inside Haskell, with higher level semantics and cleaner syntax, while still offering competitive performance.

Thus, the motivations for this thesis is to explore the feasibility of implementing a neural

network in a more on-the-fly, user-friendly approach using Accelerate. If successful, it may enable us test neural network hypotheses in a more convenient manner.

As an initial prototype, a feed-forward back-propagation (FFBP) neural network implementation has recently been made [Eve16].

This project aims to build upon that work and create a convolutional neural network (ConvNet), which is often specialised for image recognition problems.

It is crucial that the performance of the implementation is fairly competitive to existing high-level language implementations of neural networks, such as Python. Thus ways to enhancing the performance will also be explored once the basic implementation is finished.

The following section, Chapter 2 outlines the background relating to this topic, from a general overview of neural networks, the mathematics behind FFBP algorithm, an overview of the Accelerate language to previous implementation using Accelerate.

Chapter 3 introduces my thesis proposal and predicts some issues as well areas that need further development.

Finally, Chapter 6 summarises the contents of this report.

Chapter 2

Background and Related Works

2.1 Neural network architecture

Broadly speaking, a neural network can be described as a certain layering of nodes, or *units*, connected to each other by directed *links*, where each link has a certain numeric weight that signifies the strength of connection between the connected nodes.

Historically, the concept of ‘net of neurons’ whose interrelationship could be expressed in propositional logic was first proposed by [MP43] in 1943, inspired by a “all-or-none” behaviour of the biological nervous system. The first basic unit, also called the *perceptron*, was invented by [Ros62]. A perceptron will be activated if the sum of all the input values from its input links, say x_1, \dots, x_m , multiplied by the links’ corresponding weights, say $\theta_1, \dots, \theta_m$, is above that unit’s certain threshold value, or *bias* b , such that

$$\text{output} = \begin{cases} 0 & \text{if } \sum_{i=1}^m x_i \theta_i \leq b \\ 1 & \text{otherwise} \end{cases}$$

The above is equivalent to vectorizing the inputs to $\mathbf{x} = [x_1, \dots, x_m]$, weights to $\boldsymbol{\theta} =$

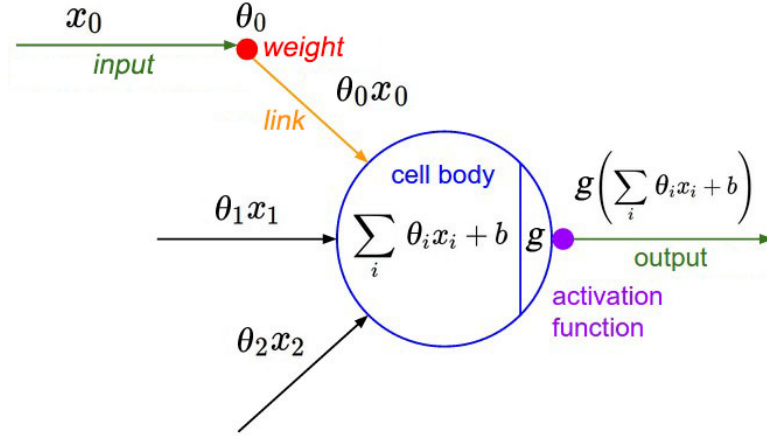


Figure 2.1: Structure of a modern unit by [Kar16].

$[\theta_1, \dots, \theta_m]$ and inverting the sign on b , so that,

$$\text{output} = \begin{cases} 0 & \text{if } \mathbf{x} \cdot \boldsymbol{\theta} + b \leq 0 \\ 1 & \text{otherwise} \end{cases}$$

The perceptron eventually evolved into the modern unit, which computes the output value as a *range* of values, obtained by applying an *activation function* to the sum of its inputs and bias. With this modification, a small change in the inputs only resulted a small change in the output, allowing a more convenient way to gradually modify the weights and consequently, improve the learning algorithm [Nie15].

There are various activation functions; historically, the most commonly used is the *sigmoid* function, $\sigma(x) = 1/(1 + e^{-x})$. Its advantages and disadvantages are outlined in 2.5. [Kar16] recommends using less expensive functions with better performance, such as,

1. Tanh function, $\tanh(x) = 2\sigma(2x) - 1$.
2. Rectified Linear Unit (ReLU) function, $f(x) = \max(0, x)$.
3. Leaky ReLU function, $f(x) = 1(x < 0)(\alpha x) + 1(x \geq 0)(x)$
4. Maxout function, $\max(w_1^T x + b_1, w_2^T x + b_2)$.

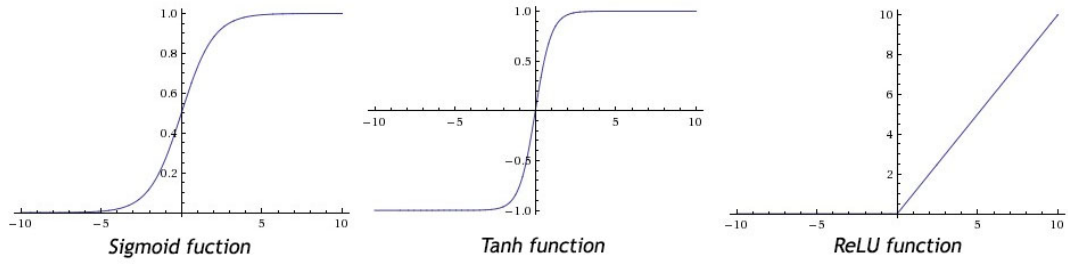


Figure 2.2: Graphs of some common activation functions [Kar16].

A unit’s output can be expressed as $g(\mathbf{x} \cdot \boldsymbol{\theta} + b)$, where $g(x)$ is the chosen activation function.

As previously mentioned, the general architecture of a neural network can be described as distinct layers of these units, which are connected to units in its adjacent layers. The most common layer type is *fully-connected*, which means that each unit in a layer is connected to every unit in the adjacent layer [Nor14].

The *input layer* receives input values corresponding to the number of features¹ in the neural network. The last, or *output layer* usually corresponds to different classes in a multi-classification problem, or some real-valued target in a regression problem [Kar16]. The layers in between input and output layers are called *hidden layers*; a neural network is classified as DNN if it contains more than one hidden layer. Increasing the size and numbers of hidden layers also increases the *capacity* of the neural network [Kar16]; that is, the space of its representable functions. However, this may undesirably result in *overfitting*².

There are numerous neural network classifications depending on their architecture; the design relevant to this thesis is *supervised*³ FFBP neural network. Its training process

¹For instance, in a 200×200 pixel image recognition problem, there may be 40,000 features corresponding to each individual pixel’s RGB values.

²Overfitting refers to modeling the learning algorithm to excessively fit to the training samples. It thereby increases the risk of including unnecessary noise in the data, resulting in more inaccurate model.

³As in “supervised learning”, a concept in machine learning where a set of training examples is paired up with a set of corresponding desired output values. A supervised

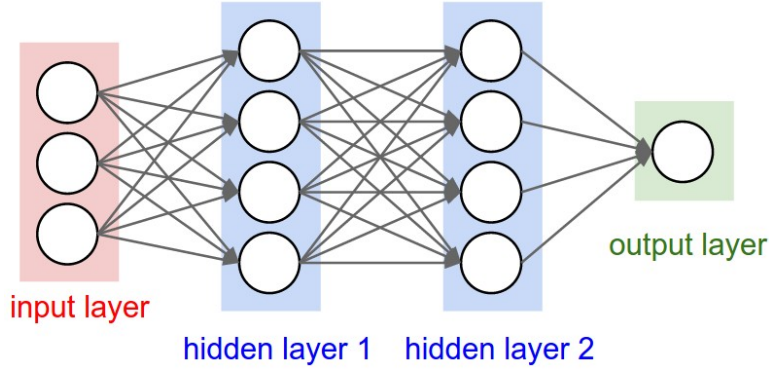


Figure 2.3: An example of a 2-layer neural network [Kar16].

and mathematical representation are briefly outlined in 2.2.

Finally, [Nor14] summarises the attractiveness of neural networks as follows:

1. Its capacity to support parallel computation.
2. Its fault tolerant nature against novel inputs.
3. *Graceful degradation*, which means a gradual performance drop-offs in worsening conditions.
4. The usage of inductive learning algorithms to train the networks.

2.2 Feed-forward back-propagation learning algorithm

This section explains the mechanics and the mathematical representation involved in training a fully-connected, supervised FFBP neural network, based on the works in [Ng16]. Given a set of features and training samples, this learning algorithm aims to find the correct weight distribution in the neural network in two stages: *feed-forward propagation* and *back-propagation*.

neural network thus adjusts its links' weights to get the correct output values during its training phase.

First, the weights are randomly initialised within the permitted range of the chosen activation function. For example, this range is $[0, 1]$ for a sigmoid function; for a tanh function, it is $[-1, 1]$.

Now, in a k -layer neural network, let the size or the number of units in layer j be denoted as $|j|$. Let a particular training sample, s , be denoted as $(\mathbf{x}^{(s)}, \mathbf{y}^{(s)})$, such that $\mathbf{x}^{(s)} = [x_1^{(s)}, \dots, x_m^{(s)}]$ is the sample input and $\mathbf{y}^{(s)} = [y_1^{(s)}, \dots, y_n^{(s)}]$ is the matching desired output. Let $a_i^{(j)}$ be the activation value of unit i in layer j , where $1 \leq i \leq |j|$, $1 \leq j \leq k$. Let $g(x)$ be the activation function; $\Theta_{qp}^{(j)}$ be the weight of a link from unit p in layer j to unit q in layer $j+1$; and, let $\Theta^{(j)} = [\Theta_{qp}^{(j)}]$ for $1 \leq q \leq |j+1|, 1 \leq p \leq |j|$ be the matrix of weights controlling function mapping from layer j to $j+1$.

Then we can express $a_i^{(j)}$ as,

$$a_i^{(j)} = g(\Theta_{i1}^{(j-1)} a_1^{(j-1)} + \Theta_{i2}^{(j-1)} a_2^{(j-1)} + \dots + \Theta_{i|j-1|}^{(j-1)} a_{|j-1|}^{(j-1)}) \quad (2.1)$$

For instance, the activation of unit i in the first hidden layer can be expressed as,

$$a_i^{(2)} = g(\Theta_{i1}^{(1)} x_1^{(s)} + \dots + \Theta_{im}^{(1)} x_m^{(s)})$$

and, in the output layer as [Ng16],

$$a_i^{(k)} = g(\Theta_{i1}^{(k-1)} a_1^{(k-1)} + \dots + \Theta_{i|k-1|}^{(k-1)} a_{|k-1|}^{(k-1)})$$

Also, unlike the approach taken above by Ng (2016), [Kar16] states that the activation function is not commonly applied to output layer, because often the result as a real-value number received by the outer layer is the information sought by the user.

2.1 can be simplified using vectorised implementation. Let the activated units in layer j be denoted as $a^{(j)} = [a_1^{(j)}, \dots, a_{|j|}^{(j)}]$. Then inputs to this layer can be expressed as $z^{(j)} = \Theta^{(j-1)} a^{(j-1)}$ and so $a^{(j)}$ becomes,

$$a^{(j)} = g(z^{(j)}) \quad (2.2)$$

Forward-propagation process ends when the input values are thus propagated to the output layer.

Next, back-propagation involves re-distributing the error value between the expected output, $\mathbf{y}^{(s)}$, and actual output, $a^{(k)}$, back from the output layer through the hidden layers [RHW86]. This concept is based on the idea that the previous layer is responsible for some fraction of the error in next layer, proportional to the links' weights.

Let $\delta_i^{(j)}$ denote the error value in unit i in layer j and $\delta^{(j)} = [\delta_1^{(j)}, \dots, \delta_{|j|}^{(j)}]$ be the vectorised error values. Then, for $1 < j < k$,

$$\delta^{(j)} = (\Theta^{(j)})^T \delta^{(j+1)} \cdot * g'(z^{(j)}) \quad (2.3)$$

where $*$ is an element-wise multiplication. The error in the output layer is $\delta^{(k)} = a^{(k)} - \mathbf{y}^{(s)}$ and that there is no error in the first layer, because as input values, they cannot contain error.

Finally, the error in link weight $\Theta_{qp}^{(j)}$ is denoted as $\Delta_{qp}^{(j)}$, such that,

$$\Delta_{qp}^{(j)} = a_p^{(j)} \delta_q^{(j+1)}$$

This, too, can be simplified using vectorised implementation as,

$$\Delta^{(j)} = \delta^{(j+1)} (a^{(j)})^T \quad (2.4)$$

Back-propagation ends for s when the errors from the output layer is propagated to the first hidden layer.

The FFBP learning algorithm is then repeated for all the training samples. $\Delta^{(j)}$ accumulates all the errors in the training set during this process. Once the process is finished, the final values are averaged out by the size of the training set, a *regularisation term* is added, and finally the weights are updated. A regularisation term is a value that is added in gradient descent algorithm in machine learning, to prohibit features that are vastly different in its range of input values from one another from distorting the results [Ng16]. This entire process is also known as a form of *batch gradient descent* (BGD) learning algorithm in machine learning [Ng16].

There are other advanced optimization methods that can improve the performance of neural networks, but these have yet to be explored at the time of this report. As

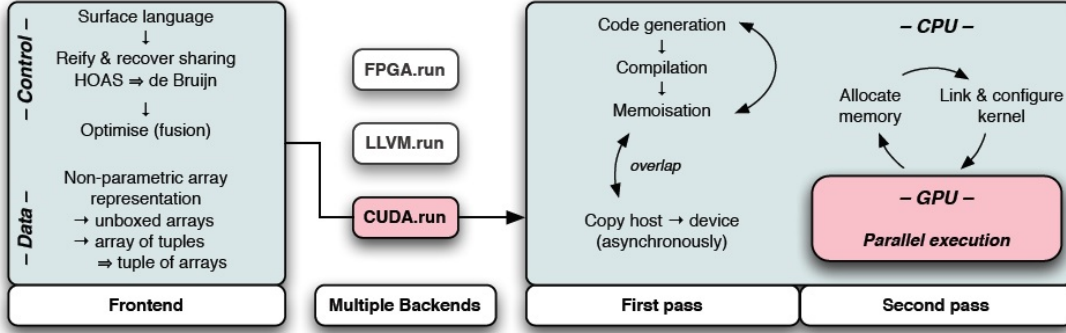
with other machine learning algorithms, the performance may also be improved with either altering various parameters, such as regularisation parameter λ and the learning rate parameter α , altering the number of features, gaining more training examples, adding polynomial features, or any combination of these [Ng16]. However, *diagnostic analysis* is often the fastest and most economically sound method to determine which set of features is effective [Ng16]. Diagnostic analysis is a form of trial-and-error testing of features sets, or *hypotheses*, with a small set of training examples to assess its performance and thus its suitability.

2.3 GPU-accelerated programming and neural networks

Neural networks implemented with GPU-accelerated programming have shown a significant performance improvement. For instance, [OJ04] had a 20-fold performance enhancement of a multi-layered perceptron (MLP) network to detect text using an ATI RADEON 9700 PRO in 2004. More recently, [GdAF13] showed that performance gains from parallel implementation of neural networks in GPUs are scalable with the processing power of the GPU used. Their results show that performance enhancement over the pure CPU implementation increased with data set size before reaching a plateau, a limit which they contribute to the saturation of the GPU's processing cores.

[NVI14] explains that GPU computing is particularly well-suited to neural networks due to its massively parallel architecture, consisting of tens of thousands of cores. Thus, as single GPUs can hold entire neural network, they state that neural networks benefit from an overall bandwidth increase, reduction in communication latency, and a decrease in size and power consumption compared to a CPU cluster. Furthermore, as neural network units essentially repeat the same computation only with differing input values, the algorithm complements the GPU architecture as there is minimal need for conditional instructions that could trigger thread divergences, which can dramatically reduce the GPU throughput.

The main GPU programming language is CUDA, an API model created by NVIDIA

Figure 2.4: Structure overview of `Data.Array.Accelerate`. [CKL⁺11]

in 2007. It has a C/C++ language style and the added benefits that it bypasses the need to learn graphics shading languages or learn about computer graphics in order to program the GPU. The alternative to CUDA is Open Computing Language (OpenCL) released in 2009; also based on C/C++, it is considered to be the more complicated language of the two, but with enhanced portability. As both languages are very low-level [Mar13], there is a need for a way to create, manipulate and test neural networks in less complicated, more user-friendly, safer, higher-level language, such as a functional language.

2.4 Accelerate

Accelerate is an Embedded Domain-Specific Language (EDSL) for GPU programming, released by UNSW PLS in 2011. EDSLs are restricted languages that are embedded in a more powerful language, so as to reuse the host language’s infrastructure and enable powerful metaprogramming. In the case of Accelerate, Haskell is the host language and it compiles into CUDA code that runs directly on the GPU.

Accelerate provides a framework for programming with arrays [Mar13] – Accelerate programs take arrays as input and output one or more arrays. The type of Accelerate arrays is,

```
data Array sh e
```

where `sh` is the *shape*, or dimensionality of the array, and `e` is the *element type*, for

```

data Z          = Z
data tail :: head = tail :: head

type DIM0 = Z
type DIM1 = DIM0 :: Int
type DIM2 = DIM1 :: Int
type DIM3 = DIM2 :: Int

type Array DIM0 e = Scalar e
type Array DIM1 e = Vector e

```

Figure 2.5: Types of array shapes and indices [CKL⁺11].

instance `Double`, `Int` or tuples. However, `e` cannot be an array type; that is, Accelerate does not support nested arrays. This is because GPUs only have flat arrays and do not support such structures [Mar13].

Types of array shapes and indices are shown in Fig. 2.5 [CKL⁺11]. It shows that the simplest shape is `Z`, which is the shape of an array with no dimensions and a single element, or a scalar. A vector is represented as `Z :: Int`, which is the shape of an array with a single dimension indexed by `Int`. Likewise, the shape of a two-dimensional array, or matrix, is `Z :: Int :: Int` where the left and right `Int`s denotes the row and column indexes or numbers, respectively.

Common shapes have type synonyms, such as scalars as `DIM0`, vectors as `DIM1` and matrices as `DIM2`. Similarly, common array dimensions of zero and one also have type synonyms as `Scalar e`, `Vector e`, respectively.

Arrays can be built using `fromList`; for instance, a 2×5 matrix with elements numbered from 1 to 10 can be created with,

```
fromList (Z::2::5) [1..] :: Array DIM2 Int
```

To do an actual Accelerate computation on the GPU, there are two options [Mar13]:

1. Create arrays within the Haskell world. Then, using `use`, inject the array `Array a` into the Accelerate world as `Acc (Array a)`. Then, use `run`.

```

-- build an array in Haskell world
fromList :: (Shape sh, Elt e) => sh -> [e] -> Array sh e

-- to execute an Accelerate computation on the GPU
run :: Arrays a => Acc a -> a

-- inject Haskell world array into Accelerate world
use :: Arrays arrays => arrays -> Acc arrays

-- create an array in Accelerate world (array filled with user-specified
  function)
generate :: (Shape ix, Elt a)
  => Exp ix -> (Exp ix -> Exp a) -> Acc (Array ix a)

-- create an array in Accelerate world (array filled with same values)
fill :: (shape sh, Elt e) => Exp sh -> Exp e -> Acc (Array sh e)

```

Figure 2.6: Some Accelerate functions [Mar13].

2. Create arrays within the Accelerate world. There are various methods, such as using `generate` and `fill`. Then, use `run`.

`run` executes the Accelerate computation and copies the final values back into Haskell after execution. In `Acc a`, `Acc` is an Accelerate data structure representing a computation in the Accelerate world, that yields a value of type `a` (more specifically, an array) *once it executes* [McD13, Mar13].

Now, as the first method may require the array data to be copied from computer’s main memory into the GPU’s memory, the second method is generally more efficient [Mar13]. All the aforementioned functions are outlined in Fig. 2.6.

Further details about the Accelerate language is continued in 2.5.

2.4.1 Advantages of Accelerate

There are several advantages to using Accelerate. First, it results in much simpler source programs as programs are written in Haskell syntax; Accelerate code is very similar to an ordinary Haskell code [Mar13]. For instance, Fig. 2.7 shows a dot product function

```

-- dot product in Haskell
dotp :: [Float] -> [Float] -> Float
dotp xs ys = foldl (+) 0 (zipWith (*) xs ys)

-- dot product in Accelerate
dotp :: Acc (Vector Float) -> Acc (Vector Float) -> Acc (Scalar Float)
dotp xs ys = fold (+) 0 (zipWith (*) xs ys)

```

Figure 2.7: Haskell and Accelerate versions for dot product [McD13].

comparison in Haskell and in Accelerate by [McD13]. There are minimal syntactic difference; for example, in the input and output types (Haskell’s version takes and gives Haskell arrays while Accelerate’s `dotp` deals with only Accelerate arrays), and in that Haskell’s `foldl` is a left-to-right traversal, whereas Accelerate’s `fold` is neither left nor right as it occurs in parallel [McD13].

Second, as Accelerate is embedded in Haskell, it can benefit from inheriting Haskell’s functional language characteristics. For instance, Haskell as a pure language is advantageous for parallel computations as it will prohibit side effects that can disrupt other threads; and, GPUs particularly require an extremely tight control flow due to massive numbers of threads that are generated. Another Haskell characteristic is having a more powerful type system, which could enforce a stronger checking for certain properties – thereby catching more errors – at compile time. An example of this is the use of types `Acc` and `Exp`, which separates array from scalar computations and prevents many cases of nested data parallelism, which is unsupported in Accelerate.

Finally, Accelerate is a dynamic code generator [CKL⁺11] and as such it can,

- Optimise a program at the time of code generation simultaneously by obtaining information about the hardware capabilities.
- Customise the generated program to the input data at the time of code generation.
- Allow host programs to “generate embedded programs on-the-fly”.

On the other hand, the disadvantages of using Accelerate over CUDA are the extra

overheads, which may originate at runtime (such as runtime code generation) and/or at execution time (such as kernel loading and data transfer) [CKL⁺11].

Some of the overheads however, such as dynamic kernel compilation overheads, may not be so problematic in heavily data- and compute-intensive programs, because the proportion to the total time taken by the program may become insignificant [CKL⁺11]; and, neural networks certainly fit in such a category of programs. Accelerate also uses a number of other techniques to mitigate the overheads, such as fusion, sharing recovery, caching and memoisation of compiled GPU kernels [CKL⁺11].

In terms of performance, Accelerate can be competitive with CUDA depending on the nature of the data input and the program [MCKL13].

2.5 Previous Implementations in Accelerate

A neural network in Accelerate is a fairly new concept and as such, there is only one known work in [Eve16]. In it, Everest (2016) implements a FFBP neural network with a *stochastic gradient descent* (SGD) learning algorithm. This section briefly covers the details of this implementation.

SGD algorithm is a modification of BGD algorithm, shown in 2.2. Rather than adjusting the neural network parameters after going through the entire training set, SGD updates the parameters immediately after doing the FFBP algorithm for a single training example, which is picked at random [Ng16]. As such, SGD is computationally less expensive than the BGD, and allows the training algorithms to scale better to much larger training sets [Ng16]. The disadvantages of SGD are that it is less accurate than BGD, and that it may take longer to reach the local/global minima.

The activation function is the sigmoid function. This function is mathematically convenient, because its gradient, $\sigma'(x)$, is easy to calculate:

$$\sigma'(x) = \sigma(x) \cdot (1 - \sigma(x))$$

The sigmoid function suffers from the following two disadvantages and is now mostly unused [Kar16]:

1. When the unit’s activation *saturates* at either tail of 0 or 1, the gradient of the sigmoid function nears zero (refer to the sigmoid function graph in Fig. 2.2). Zero gradients effectively ‘kill’ any signal flows through the neuron in forward- and back-propagation. Thus saturated neurons results in a “network [that] will barely learn” [Kar16]. Accordingly, extra care must be taken not to initialise the weights with a large value.
2. The range of the sigmoid function is not centered around zero. Hence if the inputs are always positive, it could introduce an undesirable *zig-zagging dynamics* in the gradient updates for weights, as the gradient on the weights will be either all positive or all negative during back-propagation. However, this is a minor inconvenience as its impact is automatically mitigated in a BGD by the time the weights are updated.

The third interesting observation is how Accelerate was utilised in this implementation. First, there are six key Accelerate functions that were used and their names and operations are listed in Fig. 2.8.

`Exp` is another Accelerate data structure, that is similar to `Acc` (refer to 2.4), but instead of an array, it represents an embedded *scalar* computation [CKL⁺11]. Functions `lift` and `unlift` are used to inject and extract a value into and out of `Exp`, respectively, and are thus essential in interpreting the indices of arrays in Accelerate [Mar13].

Two support functions were also created to assist forward- and back-propagation processes – `mvm` and `cross` (see Fig. 2.9). In `mvm`, `h` first stores the row number of the matrix input using `unlift`. The vector input, `vec` is then replicated `h` times across the first dimension using `replicate`. The resulting matrix is then element-wise multiplied with `mat` using `zipWith`. Lastly, the values of the matrix are summed and flattened back into a vector using `fold`.

```

-- apply supplied function element-wise to corresponding elements of two
  input arrays to produce a third array
zipWith :: (Shape ix, Elt a, Elt b, Elt c)
  => (Exp a -> Exp b -> Exp c)
  -> Acc (Array ix a) -> Acc (Array ix b) -> Acc (Array ix c)

-- map function within the Accelerate world
map :: (Shape ix, Elt a, Elt b)
  => (Exp a -> Exp b) -> Acc (Array ix a) -> Acc (Array ix b)

-- replicate an array across one or more dimensions according to the
  first argument (a generalised array index)
replicate :: (Slice slx, Elt e)
  => Exp slx -> Acc (Array (SliceShape slx) e)
  -> Acc (Array (FullShape slx) e)

-- reduce the innermost dimension of an array
fold :: (Shape ix, Elt a)
  => (Exp a -> Exp a -> Exp a) -> Exp a
  -> Acc (Array (ix::Int) a) -> Acc (Array ix a)

-- wraps a value in Exp
lift :: Z::Exp Int::Exp Int -> Exp (Z::Int::Int)

-- deconstruct Exp, get the structured value from within
unlift :: Exp (Z::Int::Int) -> Z::Exp Int::Exp Int

```

Figure 2.8: Key Accelerate functions used in [Eve16].

```

-- matrix vector multiplication function
mvm :: (Elt a, IsNum a)
  => Acc (Matrix a) -> Acc (Vector a) -> Acc (Vector a)
mvm mat vec
  = let Z::h::_ = unlift (shape mat) :: Z::Exp Int::Exp Int
    in A.fold (+) 0 $ A.zipWith (*) mat (A.replicate (A.lift (Z::h::All)) vec)

-- vector multiplication function
cross :: Acc (Vector Float) -> Acc (Vector Float) -> Acc (Matrix Float)
cross v h = A.zipWith (*) (A.replicate (lift (Z::All::size h)) v)
  (A.replicate (lift (Z::size v::All)) h)

```

Figure 2.9: Support functions for forward- and back-propagation used in [Eve16].

```

-- back-propagation part of backprop function
nabla_b_final = A.zipWith (*) ( costDerivative (P.last activations) y)
                                     (A.map sigmoid' (P.last zs) )
nabla_w_final = cross nabla_b_final ( P.last (P.init activations) )

...

```

Figure 2.10: Accelerate and Haskell code are mixed in [Eve16].

The process is similar in `cross`. `cross` is a vector multiplication function that returns a matrix. First, vector `v` is replicated $|h|$ number of times in the second dimension, whereas vector `h` is replicated $|v|$ number of times in the first dimension. The resulting two matrices are then element-wise multiplied using `zipWith`.

The actual FFBP algorithm is in the function `backprop`. In `backprop`, Accelerate code (imported as `A`) seamlessly interweaves with the Haskell part (imported as `P`), as seen in Fig. 2.10.

At the time of this report, Everest (2016) has reported some performance issues with this implementation, but has yet to determine the cause. He noted that the implementation was running at a slower speed than an equivalent neural network that was implemented with Theano. Theano is a Python library that is optimised for multi-dimensional array computations.

2.6 Measuring performance

One of the issues that has been raised during Thesis A is the need to find a suitable test subject, that provides an appropriate complexity, size and number to fully evaluate the performance of the implementation.

Currently, I have tentatively decided to test the system with the basic National Institute of Standards and Technology (MNIST) data set of handwritten digits. Should this prove unsuitable as a test subject, I may try an online repository for image data sets at the University of California, Irvine Center for Machine Learning and Intelligent Systems.

Another problem that I may encounter using such pre-made repositories is that there may be insufficient training samples in the provided data set to train my neural network. In machine learning, a concept called *artificial data synthesis* may resolve this dilemma [Ng16].

Artificial data synthesis comprises of the following two methods to create *synthetic data*:

1. Create new *labeled* samples by superimposing original sample with a suitable replacement. For example, an original image of an alphabet can be edited to a new sample by overlaying the existing letter with a new font type of the same letter.
2. Amplify the data set by introducing *smart* distortion to original sample. For instance, edit an original image of an alphabet into multiple versions by introducing various wave-like distortions.

Artificial data synthesis is generally more efficient than obtaining raw data and labeling them manually. In the second method, the distortion must be non-trivial and the resulting sample must lie within a naturally occurring variance – it must be reasonably found in the real world [Ng16].

Chapter 3

Implementation

3.1 Matlab implementation of neural network

There are several motivations for choosing this particular implementation of neural network as a reference point. First, Matlab implementation is heavily reliant upon the mathematical interpretation of neural network and is clearly understandable where matrix multiplication and vectorisation is concerned. It was projected that it would be fairly simple and in the closest in spirit implementation to how it may work in Accelerate due to this.

Secondly, the Matlab implementation had a certain data set with expected 'answers' to compare my own implementations to. Thus, I could be assured that my implementation in Accelerate was accurate enough to be reliable, particularly in the light of difficulty of debugging Accelerate programs. Passing this 'accuracy' test will prove the small network reliable enough to be built upon for further development in the future.

Thirdly, the codebase that I am basing my program is from Coursera, an online self-learning course, made by Andrew Ng of Stanford University. This course has drawn wide praise for its material and presumed to be reviewed by many in the same field. The structure of the course is reliable in terms of correctness and efficiency, and imple-

mented already with much knowledge in the field. Hence, I projected that the Matlab implementation would be optimised for the best performance.

Lastly, in terms of familiarity, I was more conversed with Matlab than with other neural network implementations, such as Python, C++, or Haskell, (PUT REFERENCES TO THESE IMPLEMENTATIONS) which may needlessly increase the time to start the project. I had researched about other implementations, but found that it took more time to understand these in order to integrate or implement an Accelerate neural network.

TO CHECK::::: Can C++ or Python versions use multiple threads/GPU?

3.1.1 Brief characteristics of Matlab

MATLAB, or Matrix Laboratory, is a highly domain-specific programming language, specialised to conduct numerical calculations and analysis in late 1970s. It is an imperative, object-orientated, procedural language. It is widely used among the industry and academia, particularly in science, engineering and economics.

MATLAB is a weakly typed programming language, as types are implicitly converted [Unk17]. This means that variables can be declared without an explicit declaration of their type. Furthermore, MATLAB is also dynamically typed, meaning that the types may also change during runtime. All variables in MATLAB are "structure arrays", that is, each element of the array have the same fields.

MATLAB functions accept matrices as an argument, and will automatically apply multiplications of a scalar to each element of the matrix as in Accelerate's `zipWith`. As a result, MATLAB code is deceptively simple and does not reveal the actual structure of the underlying operation. Indexing of matrices and arrays also start from 1. Method dispatching also does not strictly adhere to the method signature, but selects the method by first matching the arguments in a class precedence and then by left-most priority [Mat17]. However, MATLAB also does not support overloading functions of the same name using different signature of the same name.

3.1.2 Neural network structure

MATLAB neural network is a 3-layer simple neural network - input layer, hidden layer and an output layer. There is an bias unit which always outputs +1 in each layer to the next. My implementation can easily be modified to take more than 1 hidden layer by changing `nnCostFunction`. Hidden layer in this case roughly corresponds to detectors that look for strokes and other patterns in the input [Ng16].

3.2 Accelerate Implementation

The parts to Matlab program can be preportioned into 3 equations, and I will briefly outline how they have been implemented in the sections following:

1. Initialisation of parameters
2. Neural network cost function
3. Function minimise conjugate gradient function

3.2.1 Initialisation

Initialisation is a straightforward process, where values of alphas, randomisation of weight vectors are set. For effective random initialisation, theta values should be in the range $[-\epsilon_{init}, \epsilon_{init}]$ where one effective choice of ϵ_{init} is,

$$\epsilon_{init} = \sqrt{6}/\sqrt{L_{in} + L_{out}}$$

where L_{in} is number of units in the preceding layer, and L_{out} is the number of units in the subsequent layer of the theta/weights.

There is no optimal λ , or learning rate value. Generally, the one that gives the best result for the given data set is determined by trial-and-error. Likewise, the number

of hidden units and even the number of hidden layers also seems to be determined by trial-and-error.

The numbers for the input and output units correspond to the number of attributes in the samples and the number of classifications that these samples should be divided into.

3.2.2 Neural network cost function

This function implements both the feed-forward and back-propagation to a sample data input in the existing neural network system and updates the weight vectors and error costs accordingly. It includes application of sigmoid function and regularisation calculation.

However, instead of parsing each sample data one-by-one, following the style of MATLAB implementation, it groups all of the sample data into one massive matrix to parse them in all at once in bulk.

CHECK IF THIS IS CORRECT:: Although this batch sample method is less accurate than if the examples were parsed in one by one, it is much more time efficient.

The Accelerate implementation of this was also straightforward as this function only requires reshaping of the vectors, implemented using `reshape`, matrix multiplications, at first using `mmult`, eventually replaced with `INSERT NAME OF NEW MATRIX MULTIPLIER HERE` which has better performance. Other arithmetic operations were applied to matrixes coupled with `map` and `zipWith`.

As Accelerate has its own sets of arithmetic operations, any calculations that were needed in the Accelerate world was using the Accelerate version, marked with `A`. The Haskell world version was marked with `P` for `Prelude`.

PUT EXAMPLE HERE

For the full functions, please refer to Appendix 1 3.1, 3.2

```

function [J grad] = nnCostFunction(nn_params, input_layer_size, hidden_layer_size, num_labels, X, y, lambda)

% Reshape nn_params/theta vector into matrix theta1 and theta2
Theta1 = reshape(nn_params(1:hidden_layer_size * (input_layer_size + 1)), hidden_layer_size, (input_layer_size + 1));

Theta2 = reshape(nn_params((1 + (hidden_layer_size * (input_layer_size + 1))):end), num_labels, (hidden_layer_size + 1));

% Setup some useful variables
m = size(X, 1);
num_labels = size(Theta2, 1);

% Feed-forward
a1 = [ones(1, m); X'];
z2 = Theta1 * a1;
a2 = [ones(1, m); sigmoid(z2)];
a3 = sigmoid(Theta2 * a2);

% Convert vector y into matrix Y, s.t. forall m=1:m, Y[m][i] = 1, 0 otherwise
Y = zeros(num_labels, m);
for i=1:size(X)
    Y(i,y(i)) = 1;
end

% Compute regularized cost
J = (1/m) * sum(sum(-Y .* log(a3) - (1 - Y) .* log(1 - a3)));
J = J + (lambda / (2*m)) * sum(sum(Theta1(:, 2:end) .^ 2));
J = J + (lambda / (2*m)) * sum(sum(Theta2(:, 2:end) .^ 2));

% Backpropagate to get gradient information.
d3 = a3 - Y;
d2 = (Theta2' * d3) .* [ones(1, m); sigmoidGradient(z2)];

Theta2_grad = (1/m) * d3 * a2';
Theta1_grad = (1/m) * d2(2:end, :) * a1';

% Add gradient regularization
Theta2_grad = Theta2_grad + (lambda / m) * ([zeros(size(Theta2, 1), 1), Theta2(:, 2:end)]);
Theta1_grad = Theta1_grad + (lambda / m) * ([zeros(size(Theta1, 1), 1), Theta1(:, 2:end)]);

% Reshape gradients into single vector
grad = [Theta1_grad(:) ; Theta2_grad(:)];

end

```

Figure 3.1: Neural network cost function in Matlab.

```

158 nnCostFunction ::
159     Acc (Vector Float)           -- input flattened thetas vector
160     -> Exp Int                   -- input layer num
161     -> Exp Int                   -- hidden layer num
162     -> Exp Int                   -- num of labels
163     -> Acc (Matrix Float)        -- X (data matrix) in the form [1 X] (5000x401)
164     -> Acc (Vector Float)        -- y (labels)
165     -> Exp Float                 -- lambda
166     -> Acc (Scalar Float, Vector Float) -- j, theta1+theta2 vector
167 nnCostFunction ts l1 l2 n xs y lambda =
168     let
169         Z :: h :: w = unlift (shape xs) :: Z :: Exp Int :: Exp Int
170
171         -- unroll theta1
172         theta1 = reshape (index2 l2 (l1+1)) $ A.take (l2*(l1+1)) ts
173         theta2 = reshape (index2 n (l2+1)) $ A.drop (l2*(l1+1)) ts
174
175         -- make vector y into matrix Y
176         ys = matrixfy y
177
178         -- feedforward
179         a3 :: Acc (Matrix Float)
180         a1 = xs
181         z2 = mmult theta1 (transpose a1)
182         a2 = (fill (lift (Z :: h :: constant 1)) 1 :: Acc (Matrix Float))
183             A.++ (A.transpose $ A.map sigmoid z2)
184         z3 = mmult a2 (A.transpose theta2)
185         a3 = A.map sigmoid z3
186
187         -- calculate cost J
188         j :: Acc (Scalar Float)
189         j = A.zipWith (+) regCost
190             $ A.map (\x -> x / A.fromIntegral h)
191             $ A.foldAll (+) 0
192             $ A.zipWith (\y a -> -y * (log a) - (1-y)*log(1-a)) ys a3
193         where
194             regCost = A.map (\x -> x * lambda / (2*(A.fromIntegral h)))
195                     (A.zipWith (+) j1 j2)
196             j1      = foldAll (+) 0 (A.zipWith (*) ttheta1 ttheta1)
197             j2      = foldAll (+) 0 (A.zipWith (*) ttheta2 ttheta2)
198
199         ttheta1 = A.tail theta1
200         ttheta2 = A.tail theta2
201
202         -- backpropagate to get gradients
203         d3 = A.zipWith (-) a3 ys
204         d2 = A.zipWith (*)
205             (mmult d3 theta2)
206             ((fill (lift (Z :: h :: constant 1)) 1 :: Acc (Matrix Float))
207              A.++ (A.transpose $ A.map sigmoidGradient z2))
208
209         theta2grad = A.map (\x -> x/A.fromIntegral h)
210                     $ mmult (transpose d3) a2
211         theta1grad = A.map (\x -> x/A.fromIntegral h)
212                     $ mmult (transpose (A.tail d2)) a1
213
214         -- add gradient regularisation
215         theta1grad_ = A.zipWith (+) theta1grad
216                     $ A.map (\x -> lambda * x/A.fromIntegral h)
217                     ((fill (lift (Z :: w1 :: constant 1)) 0 :: Acc (Matrix Float))
218                      A.++ ttheta1)
219         where
220             Z :: h1 :: w1 = unlift (shape theta1) :: Z :: Exp Int :: Exp Int
221
222         theta2grad_ = A.zipWith (+) theta2grad
223                     $ A.map (\x -> lambda * x/A.fromIntegral h)
224                     ((fill (lift (Z :: w2 :: constant 1)) 0 :: Acc (Matrix Float))
225                      A.++ ttheta2)
226         where
227             Z :: h2 :: w2 = unlift (shape theta2) :: Z :: Exp Int :: Exp Int
228
229         grads = flatten theta1grad_ A.++ flatten theta2grad_
230
231     in
232     lift (j, grads)

```

Figure 3.2: Neural network cost function in Accelerate.

3.2.3 Function minimise nonlinear conjugate gradient function

This function is a modified version of MATLAB's `fminunc`. Given

```
= fminunc(func, x0)
```

`x` is the the local minimum of unconstrained multivariate function `func`, from starting point `x0`. `x0` can be a scalar, vector or a matrix. [Reb13]

`fmincg` is a more efficient modification of `fminunc` to minimize a continuous differentiable multivariate function. It uses Polack-Ribiere flavour of conjugate gradients, quadratic and cubic polynomial approximations and the Wolfe-Powell stopping criteria to more efficiently calculate slope and stepping sizes [Mat17]. The mathematics behind applying these methods are beyond the scope of this project.

The function terminates when it either finds the local minimum, or if the progress is so non-significant that it is not worth any further exploration. It returns the solution vector as `X` and the cost vector `fX`, which indicates the cost of each iteration or the progress made.

Translating `fmincg` into Accelerate is tricky. First, the MATLAB code had around 17 parameters, all of which constantly updated their values in a procedural way. Without a knowledge of the underlying mathematics, the procedure was puzzling. Their non-descript names, such as, `d1`, `f1`, `v1` were not enlightening either. Overall, it was difficult to follow the flow of control. I thus have followed the flow of procedure very closely, albeit with some substitutions, as there were some aspects that were not yet implemented in Accelerate, such as `isInfinite` and `isNaN`.

Second, there were three `while` loops in this code, with three `if-else` statements, one which had a flow divergence. Due to this, the type of flat parallelism may not be best suited for the GPU, although the flow divergence was upon a failure to find local minimum - which happens when the function supplied to `fmincg` is inaccurate [Reb13]. Thus, to get rid of this flow divergence, I have taken the assumption that there is always a local minimum that `fmincg` can find, because the function supplied can be checked

to be accurate prior to being supplied to this function.

Also, due to the limitations of MATLAB in `fmincg`, there is a seemingly redundant step of flattening the initial weight matrices into a vector, passing it as a parameter into `fmincg`. It is promptly then unrolled back into their original matrix shape, and after all the operations inside this function is complete, it is reflatened into a vector and returned.

This is to enable the function to iterate regardless of the matrices' size or shape. This duty is pushed to the function.

The MATLAB version of the code had approximately 175 lines. I divided these up into their `while` loops and connected the parts using Accelerate's `awhile` flow control. This required `lift`, `unlift` in order to pack and unpack the many variables into a single `Acc` tuple in order to be passed around the loop. Through this process, I found that Accelerate cannot infer the type unless if the `unlifted` expression is used, and it is thus sometimes necessary to predefine types for certain terms.

Accompanying this issue was that `awhile` requires that set of results I need after the `while` loop finishes be part of the tuples wrapped in `Acc`. This meant that even the paramters that are not used needed to be packed together, and these always needed a help in type inference as Accelerate could not infer their types during the loop.

GIVE EXAMPLES

Such an implementation could be considered inefficient due to the number of space it consumes memory by creating intermediate variables rather unnecessarily in other languages. This has less impact with Accelerate due to 'sharing recovery', which will be discussed in 3.4.

3.3 Limitations of this implementation

There are several issues with my Accelerate implementation. For one, there are a couple of functions which may not cover all the cases that MATLAB implementation may cover. For example, `fmincg` requires to optimise and to take care of cases where certain variables are `isinf`, `isreal` or `isnan`. Since these are yet to be implemented in Accelerate, I have substituted them for when a determinate may be less than zero for `isreal`, divisor is 0 for `isnan` and ignored the case for `isinf`. This may not cover all the range of numbers.

Secondly, Matlab's `double` is by default a double-precision data type, and requires 64 bits [Mat17]. Yet, after testing it on the sample data, using `double` produces a result further away from the expected result than had I have had parse them in as `float` in Accelerate. This is a problem, because it may lead to inaccuracy. Also, one part in the MATLAB code accounts for overflow it seems, by minusing a `realmin` from a dividend,

– – *PUTEXAMPLEHERE*

but `realmin` for `Float` is $1.1755e - 38$ and for a `Double` is $2.2251e - 308$, which are orders of $1e270$ magnitude different.

Lastly, some of the optimisations in `fmincg` to come to the conclusion faster has been ignored, namely, the innermost loop and the handling a failure to obtain an answer. The reasons for this is that failure should not be triggered if the function input is valid and it needlessly slows down the software by introducing flow divergence. Also, the innermost loop does not behave in the expected manner and the reasons for this is still unfathomed at the time of writing the thesis.

3.4 Benefits of Accelerate implementation

Accelerate has inherent benefits.

For instance, even if the code is 'inefficient' in the sense that it has repeating parameters, by having 'sharing recovery', Accelerate will reduce the number of parameters to the bare minimum during the production of the ASTs.

Chapter 4

Results

I have used Le Cunn's handwritten digit data set to test the relative performance of MATLAB and Accelerate conversion of the code. The backend of Accelerate is `llvm` as this handset is too small to test on the GPU for now.

4.1 Performance results

The result of this work is the present document, being both a \LaTeX template and a thesis requirement specification.

4.2 Others etc

The Dual function of this document somewhat de-emphasises the primary purpose of the document, namely the thesis requirements. It would be better, if these could be stated on a few concise pages (cf Appendix 1, p34).

Chapter 5

Evaluation

This section contains the evaluation of the result and the overall significance of my thesis result in the light of project's objective.

5.1 Discussion

The result of this work is the present document, being both a \LaTeX template and a thesis requirement specification.

5.2 Incomplete works

The Dual function of this document somewhat de-emphasises the primary purpose of the document, namely the thesis requirements. It would be better, if these could be stated on a few concise pages (cf Appendix 1, p34).

5.3 Future works

Chapter 6

Conclusion

An implementation of a neural network in Accelerate may offer a convenient alternative to current CUDA or Python implementations in testing for the validity of hypotheses.

The aim of the project is to implement a ConvNet in Accelerate. ConvNet is similar to FFBP neural networks, and thus should be possible to build upon the implementation in [Eve16].

However, further research and knowledge is necessary in order to achieve this goal.

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Appendix 1

This section contains the options for the UNSW thesis class; and layout specifications used by this thesis.

A.1 Options

The standard thesis class options provided are:

undergrad	default
hdr	
11pt	default
12pt	
oneside	default for HDR theses
twoside	default for undergraduate theses
draft	(prints DRAFT on title page and in footer and omits pictures)
final	default
doublespacing	default
singlespacing	(only for use while drafting)

A.2 Margins

The standard margins for theses in Engineering are as follows:

	U'grad	HDR
<code>\oddsidemargin</code>	40 mm	40 mm
<code>\evensidemargin</code>	25 mm	20 mm
<code>\topmargin</code>	25 mm	30 mm
<code>\headheight</code>	40 mm	40 mm
<code>\headsep</code>	40 mm	40 mm
<code>\footskip</code>	15 mm	15 mm
<code>\botmargin</code>	20 mm	20 mm

A.3 Page Headers

A.3.1 Undergraduate Theses

For undergraduate theses, the page header for odd numbers pages in the body of the document is:

Author's Name	<i>The title of the thesis</i>
---------------	--------------------------------

and on even pages is:

<i>The title of the thesis</i>	Author's Name
--------------------------------	---------------

These headers are printed on all mainmatter and backmatter pages, including the first page of chapters or appendices.

A.3.2 Higher Degree Research Theses

For postgraduate theses, the page header for the body of the document is:

<i>The title of the chapter or appendix</i>

This header is printed on all mainmatter and backmatter pages, except for the first page of chapters or appendices.

A.4 Page Footers

For all theses, the page footer consists of a centred page number. In the frontmatter, the page number is in roman numerals. In the mainmatter and backmatter sections, the page number is in arabic numerals. Page numbers restart from 1 at the start of the mainmatter section.

If the **draft** document option has been selected, then a “Draft” message is also inserted into the footer, as in:

14	Draft: May 28, 2017
----	----------------------------

or, on even numbered pages in two-sided mode:

Draft: May 28, 2017	14
----------------------------	----

A.5 Double Spacing

Double spacing (actually 1.5 spacing) is used for the mainmatter section, except for footnotes and the text for figures and table.

Single spacing is used in the frontmatter and backmatter sections.

If it is necessary to switch between single-spacing and double-spacing, the commands `\ssp` and `\dsp` can be used; or there is a `sspacing` environment to invoke single spacing and a `spacing` environment to invoke double spacing if double spacing is used for the document (otherwise it leaves it in single spacing). Note that switching to single spacing should only be done within the spirit of this thesis class, otherwise it may breach UNSW thesis format guidelines.

A.6 Files

This description and sample of the UNSW Thesis \LaTeX class consists of a number of files:

<code>unswthesis.cls</code>	the thesis class file itself
<code>crest.pdf</code>	the UNSW coat of arms, used by <code>pdflatex</code>
<code>crest.eps</code>	the UNSW coat of arms, used by <code>latex + dvips</code>
<code>dissertation-sheet.tex</code>	formal information required by HDR theses
<code>pubs.bib</code>	reference details for use in the bibliography
<code>sample-thesis.tex</code>	the main file for the thesis

The file `sample-thesis.tex` is the main file for the current document (in use, its name should be changed to something more meaningful). It presents the structure of the thesis, then includes a number of separate files for the various content sections. While including separate files is not essential (it could all be in one file), using multiple files is useful for organising complex work.

This sample thesis is typical of many theses; however, new authors should consult with their supervisors and exercise judgement.

The included files used by this sample thesis are:

definitions.tex	mywork.tex
abstract.tex	evaluation.tex
acknowledgements.tex	conclusion.tex
abbreviations.tex	appendix1.tex
introduction.tex	appendix2.tex
background.tex	

These are typical; however the concepts and names (and obviously content) of the files making up the matter of the thesis will differ between theses.