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Chapter 1

Introduction

Deep learning has exploded in recent years as the forefront of what the New York Times has referred to as the “A.I. Awakening.”

< a whole lot more to go here >

AlphaGo shocked experts worldwide when, in a best of 7 series against 9-dan Go master Lee Sedol, it was able to win 4-1. Go had often been seen as an example of a problem where humans had an unsurmountable advantage. In the modern day, chess programs are able to brute force enough possibilities on a typical consumer laptop to defeat professionals. However, Go has a far more complex move space: an cursory estimate indicates that there are on the order of $19!$ possible games. Deep learning proved capable of solving the problem of judging the quality of a Go board position, which was a groundbreaking result in a field where even the best programs were unable to challenge low-ranked professionals. Surprisingly, the developers of AlphaGo noted that “AlphaGo evaluated thousands of times fewer positions than Deep Blue did in its chess match against Kasparov.” [21]

The promise of deep learning has come with additional complexities, however. Typical deep networks, while providing excellent accuracy, have far worse computational efficiency than other methods of machine learning. AlphaGo was reliant on large-scale distributed computing infrastructure in order to achieve peak performance, and in general,

< discuss performance concerns with deep learning and therefore the motivation for this thesis by optimizing that >

Chapter 2

Background

In this section, we provide a general introduction to the relevant basics of deep learning.

2.1 Neural Networks

The foundational principle of neural networks is, in its purest form, inspired by the biology of the human brain. The field of AI has often modelled new algorithms after biological phenomena; in this field, genetic algorithms are based on evolution and particle swarm optimization is based on social behaviors. The history of neural networks dates back to the beginnings of artificial intelligence research, and from those times a few fundamentals still remain.

Firstly, the structure of a basic feedforward network was established. In a general sense, a neural network is a directed graph, with neurons as nodes and weights as edges. Every neuron activates (outputs) with a strength that is a function that is the element-wise multiplication of the inputs with the edge weights. That is, if $w_{i,j}$ is the weight value between nodes i and j , n_i is the activation of node i , and N_j is the list of node indices that are connected to j , then node j will activate with strength

$$n_j = F\left(\sum_{i \in N_j} w_{i,j} n_i\right)$$

This definition relies on an activation function F , which allows the network to produce nonlinear behaviors. We can provide input into the neural network by activating a set of nodes with specific values, and we can similarly read output from any subset of nodes. A feedforward network is then any acyclic neural network. These networks are typically organized in layers of neurons, which indicate the depth of each node. In this model, layers are typically fully connected, meaning that all nodes in one layer are connected to all nodes of the next layer. This allows a computationally-efficient model of weights as a matrix M , taking input vector V to output vector MV .

Throughout modern literature, feedforward networks are an important but rarely examined component; the structure is often considered fixed and serves to provide a final classification. Key limitations to fully connected layers prevent them from being suitable for use as the sole structure of larger networks. For example, because of the fully connected nature of the layers, they require an immense amount of memory. Such a layer between two sets of just 10000 nodes would require 100

million parameters, while modern networks often have a total of 10 million parameters [7]. This extra capacity, while being inefficient, can also be bad for training in general; there is no sense of locality in such a layer, as every node is treated individually. This means that it is difficult and nearly impossible to train higher level features that should be treated equally across all areas of the input (which is of particular interest to problems like image classification).

The other key insight of neural networks is backpropagation [10], which is an algorithm to let errors accumulated from the output layer of the network propagate backwards through the network, training it in the process. As in the example above, if the network's output is O , but the correct response would be C , we can calculate the error $E = O - C$. From this, we need a cost function that determines how errors are judged; a typical example may be the L_2 loss

$$\text{Cost}(O - C) = \sum_0^n ||O_i - C_i||^2$$

However, since we know that

$$O = F\left(\sum_0^n w_i a_i\right)$$

it is possible to figure out the influence each weight had on the error by taking the partial derivative of the cost function with respect to the weight,

$$\frac{\partial \text{Cost}}{\partial a_i} =$$

Modern training methods are far more advanced, but still rely on the basic algorithm described here, which is often termed gradient descent. The main

< describe modern usage of backprop >

LeCun et al.'s seminal work in this field, *Gradient-Based Learning Applied to Document Recognition* [17], provided the first basis of using backpropagation methodologies to train visual classifiers. Even more importantly, it introduced the fundamental structure of the modern visual deep learning network. In its usage of convolutions as a method for extracting high-level features out of larger images, it set the framework for a new style of network that would prove to be far more efficient and scalable.

2.2 Convolutions

A convolution is an operator applied to two functions f and g , which provides a way of interpreting one function in the context of the other. The operation is generally defined as

$$(f * g)(t) = \int_{-\infty}^{\infty} f(r)g(t - r)dr$$

In the perspective of modern deep learning, we are primarily interested in its usage as a matrix operator; in this context, we limit the range of g to the size of the matrix s such that

$$(f * g)(t) = \int_0^s f(r)g(t - r)dr$$

In this context, we refer to g as the *convolutional kernel*. Using a convolutional kernel to preprocess the image proves to be critical to the performance of modern deep learning methods, as a small kernel can operate over a large image in parallel.

For example, we consider the basic edge-detecting matrix

$$E = \begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

This convolution will perform the element-wise matrix multiplication of the kernel E with the immediate neighbors of each pixel, then aggregate the elements by summation. That is, if the pixel values around a specific pixel e are

$$P_e = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

then the convolution at that pixel will be

$$\begin{aligned} P_e * E &= 0a + 1b + 0c + 1d - 4e + 1f + 0g + 1h + 0i \\ &= (b + d + f + h) - 4e \end{aligned}$$

Accordingly, it will create a new matrix, with each element representing the convolutional kernel applied at that point. As shown above, the convolution $P_e * E$ will have the strongest activation when there is a strong difference between the pixel e and its neighbors (b, d, f , and h), thus performing a basic localized form of edge detection. Figure 2.1 shows this convolution applied to an arbitrary image.



Figure 2.1: A demonstration of an edge-detecting convolution, from the GIMP User's Manual. [4]

A convolutional neural network is therefore the product of chaining together convolutions to perform efficient feature extraction with the standard feedforward neural network structure. LeCun's contribution to this structure was showing that the same backpropagation methods used to train other networks could also be applied to convolutional layers, allowing convolutional neural networks (CNNs) to learn their own feature extractors. This allows the CNN to determine what kinds of

high-level feature extraction is necessary for the specific problem; applying this across a variety of filters demonstrates More importantly, this allows for networks to automatically chain convolutional layers, in which the initial information can pass through multiple layers of feature extraction, which are all automatically determined from the training data.

2.3 Modern Training

While the basics of neural network training are covered above, there are significant improvements that we highlight in this section for the sake of completeness.

< talk about batch normalization, dropout, different activation functions >

2.4 Residual Networks

As network architectures have changed over time, an ongoing goal has been to develop truly deep architectures. Even as better training algorithms have allowed network depth to increase to tens of layers, it is a generally-held principle that depth, not width, is crucial for allowing a network to learn complex features. At the same time, gradient-descent methods work poorly in networks with significant depth, as the gradient term (the partial derivative of the loss function with respect to the weight) decreases significantly by each layer. This means that after a certain amount of depth in the network, the gradient is so small that it is nearly entirely noise. The issue of disappearing gradient is in some form mitigated by training methods, some of which are more heavily biased towards the sign of the gradient rather than the magnitude. However, regardless of the specific algorithm, gradients are effectively unusable for networks with significant depth for typical network architectures.

To solve this problem, He et al. [9] developed Residual Networks. The insight in this work is that typical network layers are effectively performing two tasks simultaneously—the transfer of state alongside feature extraction/classification. The former requirement necessitates that the layer learn an encoding of its input, which is inefficient. He et al. rewrite the typical neural network architecture to allow it to merely learn the latter task, and apply this as a residual (or equivalently, difference) to the inputs. That is, if a typical neural network layer takes input X , it will apply the layer L to produce $L(X)$. A residual network layer takes the input, then outputs the layer’s contribution in summation with the original input to produce $L(X) + X$. Beyond the theoretical improvements to the “task” of the layer, it is also crucially important that this identity mapping for X in a residual layer allows the gradient to propagate backwards with its original magnitude. This ensures that the gradient is present at every layer with reasonable strength, allowing the calculations for error on the specific layer operation L to be done with less noise. He et al. used this structure to produce a 152-layer network, which is almost an order of magnitude increase over previous methods. This result was enough to win ILSVRC in 2015, an industry-standard annual image classification competition, demonstrating the efficacy of the algorithm.

With regards to this thesis, residual networks have a very important property that a layer which is entirely zero (where $L = 0$) results in a layer that simply produces the identity. This means that it is easier to insert and remove residual network layers than in typical architectures. Along these lines, Huang et al. [12] introduce Stochastic Depth, which randomly drops layers during the training

phase as a form of regularization and ensuring that every layer learns something different. This is very similar to the usage of Dropout in training, except entire layers are dropped.

Further expanding on He et al.'s work, Zaguruyko and Komodakis [25] assert that residual networks are equally suited to creating wide networks as they are for deep ones; their testing indicates that it is possible to use the residual network framework effectively for networks of comparatively shallow depth (16 layers). This is of particular interest because it indicates the difficulty of determining optimal network architectures; the benefits of wide residual networks are dependent on the specific classification problem, and the

< talk about the wide varieties of residual network architectures, and how it's hard to pick the right one >

Chapter 3

Related Works

In this work, we are primarily interested in optimizing neural network architectures and other hyperparameters. Towards this end, we investigate current findings in the literature. To the best of our knowledge, neural network architecture self-optimization is a very new topic, and many results are preliminary or perhaps somewhat incomplete. Nevertheless, they provide an important glimpse into the contemporary research space, and are highly motivational to the specific topic of this thesis. The aim of this section is to cover some of the existing work that specifically focuses on network optimization, and to provide some grounding for our contributions.

3.1 Parameter Deletion

Ever since neural networks have been developed, experts have wondered how to make them more efficient. The fixed initial structure required to train a network is one that is inherently overparametrized, because the minimum number of parameters needed is not known ahead of time. Making the problem worse, neural network training is often slow and requires significant computational power, limiting the ability to test out differing numbers of parameters. The natural solution is, therefore, to train an oversized network, and to somehow whittle it down to size. Initial practices were based on heuristic deletion; that is, algorithms that deleted all weights w where $w < p$ for some low-pass filter p . These methods generally result in a sparse network (where the network has missing connections), which are difficult to represent and operate on efficiently.

LeCun et al.'s early work from 1989, *Optimal Brain Damage* [18], showed that these heuristic-based methods were inefficient and could irreparably destroy a network. He proposed a method based on error gradients that could more accurately find weights that contribute

< finish this description >

By what is effectively the butterfly effect, the deletion of a weight with small magnitude could actually prove to have a significant impact on the network.

This was taken a step further by Hassibi et al. [8] in their followup work, *Optimal Brain Surgeon*. By analyzing the Hessian matrix of the network,

< actually describe the Hessian, or do this with LeCun's example above >

Hassibi et al.'s algorithm is among the most detailed methods shown to delete weights from a network, and they show that their algorithm is in fact optimal for specific small networks. However,

the calculation of the Hessian is an $O(n^2)$ operation in both space and time, making it largely unsuitable for networks in the modern age, where n (the number of parameters) is often in the millions or tens of millions. At the same time,

Within the last few years, the literature on parameter deletion is beginning to see more activity, especially as networks grow in complexity at a pace that far outpaces the corresponding technological advancements.

< describe modern successes with using heuristic-based deletion, and some preliminary research on using optimal brain damage with large networks >

3.2 Specialized Architectures

Another key direction taken by researchers is to design the network specifically to minimize the number of parameters required. Notable work in this field includes Squeezenet [13] by Iandola et al., which utilizes a number of space-saving tricks to produce a network which has 50 times less parameters. Perhaps even more interestingly, Courbariaux and Bengio show that it is possible to constrain a network entirely to binary weights and activations (either +1 or -1) without significant loss in accuracy. They are able to construct a convolutional neural network in this way, and optimize it for CPU performance to achieve competitive results. These results are largely corroborated by Rastegari et al. [20], who also use a binarized network and significant usage of the XNOR operation to optimize a wider variety of modern networks. It is important to note, however, that the performance of these methods is still insufficient to reliably overtake GPU networks. Courbariaux and Bengio perform their training against “an unoptimized GPU kernel”, while Rastegari et al. perform an efficiency investigation but do not discuss raw performance. While such approaches show promise in the future, they are more complicated and are still far away from seeing general use in modern libraries.

On the other hand, it is not necessary to impose such harsh limits on the network in order to find areas of improvement. Google’s Inception network [23], developed by Szegedy et al., has gone through various iterations, which all involve complex pooling of different convolutional kernel sizes. In their 2016 update to the architecture [24], they focus on tuning the inefficiently large filter sizes used in the previous revision. They note that a 5×5 convolution is effectively the same (covers the same area) as two 3×3 convolutions while requiring more parameters (25 versus $9 \cdot 2 = 18$), dubbing this reduction as filter factorization. In the same vein, it is possible to reduce a 3×3 convolution to a 3×1 convolution followed by a 1×3 convolution, which requires a third less parameters.

There are various benefits to an increased number of smaller layers beyond parameter reduction. It allows the increased application of nonlinear activation functions, which are generally regarded as critical for learning complex problems. Furthermore, it allows an increased number of layers with the same number of parameters. Most networks are primarily limited by memory, especially as modern training algorithms require a Even though inference is generally more efficient, it can still remain a difficult problem for more constrained hardware; part of Squeezenet’s contribution was the possibility of reducing a model to a size that could be run on modern FPGAs.

3.3 Network Expansion

< describe early (1990s) approaches to network expansion, there's another modern paper that does a little expansion but not as interesting perhaps >

Chapter 4

Methodology

In this section, we provide a description of the algorithmic details that we propose.

4.1 Dynamic Network Capacity

Network design has almost always focused on preferring overparametrization; this principle is clear

< The network will start at a very small size, and gradually resize as error plateaus. This is a more “visible” approach to network architecture because error rates are clear and interpretable, versus the obtuse parameter of network size. >

4.2 Fixed Networks

< Some parts of the network are fixed as the network resizes. This is to prevent them from changing too significantly over time. I’m still experimenting with unfreezing these parts of the network. There’s an interesting parallel to the human brain here I believe. >

4.3 Layer-Specific Analysis

< In the residual network paper, they discuss looking at activations of each layer and investigating the standard deviations. I’m interested in using these to determine where extra layer capacity is needed; once CIFAR-100 is running, this will promptly follow. >

Chapter 5

Experiments and Results

5.1 Implementation

We performed all of our experiments within Google’s Tensorflow [1] framework. Tensorflow imposes a style of computation which is not immediately adaptable to our experiments, but it was nevertheless chosen for its prevalence and impact on current methods. Its popularity has largely affected the number of open-source code samples available, and many current architectures have clear examples in Tensorflow. The thriving ecosystem of open-source contributions around Tensorflow proved to be a highly beneficial factor in providing a variety of existing architectures for experimentation.

As was noted before, Tensorflow operates in a slightly different way than many other libraries. Rather than allowing the user to chain together operations at random, it fixes a computational graph which defines the full model. Google’s developers preferred this static model as it is generally well-suited to a lot of deep learning research, while also being flexible enough to allow distributed computing (of crucial importance to a cloud company like Google). This, however, poses an obvious problem with our algorithm, which is largely dynamic. A few workarounds had to be developed in order to interface with the static computational graph. While it is possible to use conditional blocks to disable parts of the graph, it is impossible to insert during runtime. As such, the entire possible network capacity has to be allocated upfront, which potentially reduces the range of experimentation. This additionally means that while parts of the network can be disabled, they still take important parameter space which cannot be reallocated to other parts of the network.

In his work on spatially-sparse convolutional neural networks [6], Graham noted that there are potential improvements in architecture by performing sparse convolutions. Tensorflow does not support such functionality at the moment, although it appears that they may be planning its development for the future [22]. For our experiments, we continue to rely on densely-connected networks

Other libraries were explored briefly, but they either did not provide the necessary flexibility or have a reasonable set of tutorials/examples to facilitate the work here. For example, one of the more common tools in image-based deep learning has been Caffe [14], which boasts well-tuned performance as well as a public repository of models in the Caffe Model Zoo. Unfortunately, being written almost entirely in C++, it is largely unamenable to testing and infrastructure development. Modifying Caffe to implement new training methods typically requires a significant contribution

in C++, which requires an overhead not often undertaken except by researchers with significant prior experience. Furthermore, models are loaded in a fixed format, which hampers the ability to dynamically redefine networks. On the other side of the spectrum are libraries like Keras, which usually serve as a higher-level wrapper to other deep learning libraries. They were generally judged as being insufficiently expressive for the type of modifications we performed, so we considered other options.

All experimentation was performed on a GTX 1060, which was provided via a grant from Princeton SEAS. GPU computation has widely become the standard for deep learning computation in recent years, as it can provide nearly an order of magnitude in performance. Particularly for models like modern residual networks, which can take days to converge to reasonable accuracy, it is nearly impossible to train neural networks on CPU servers. Tensorflow still utilizes the CPU extensively to coordinate training and perform a significant amount of calculations, but modern-day GPUs are nearly perfectly designed for the type of computations required for convolutions.

A recent glut of libraries aimed at helping automate the deep learning deployment process has led to a variety of different methods. NVIDIA’s CUDA and CUDNN libraries, both of which are crucial for the performance of modern deep learning libraries, require a complex set of dependencies and installation procedures. To automate this process, NVIDIA has recently released the `nvidia-docker` tool, which provides an abstraction on top of Docker that is designed to expose the GPU without requiring a complex installation method for the requisite GPU drivers. We use this library to deploy CUDNN v5, as well as the latest GPU drivers and Tensorflow version as of this writing (375.39 and 1.1.0-rc0, respectively).

As Tensorflow’s interface is best utilized in Python, we performed some initial testing with the Jupyter application. Jupyter exposes a dynamic notebook interface that allows “cells” of code to be run in an interactive instance, which also shows outputs inline. Despite being relatively useful for basic prototyping, the largely static nature of Tensorflow’s graph structure meant that for the larger tests, there was little to no developer-side improvement over traditional coding. Nevertheless, we note that Jupyter is a useful interface for demonstrating concepts, as many Tensorflow code examples online are in Jupyter `.ipynb` format. In particular, GitHub supports native inline presentation of Jupyter notebooks, which proved to be far more efficient than the typical workflow of downloading code examples, waiting for execution, and parsing terminal output which is often difficult to link to specific code sections. Jupyter is, in fact, a first-class citizen in the Tensorflow ecosystem, as it is included in the default `nvidia-docker` image provided by Google in the online Docker Hub repository.

5.1.1 Experimental Details & Notes

Throughout our experiments, we utilize the ADAM optimizer developed by Kingma and Ba [15] as it allows adaptive training without requiring the careful learning rate tuning that is generally required for straightforward gradient-descent optimization.

We also rely on Glorot and Bengio’s Xavier initializer [5], as it is a common improvement over typical random initialization that remains relatively simple to use.

We fix portions of the network by using Tensorflow’s `tf.stop_gradient` method. Support for freezing whole layers is a generally universal feature across deep learning libraries, but our investigation

showed that none supported partial freezing—that is, the ability to train part of a layer while keeping the other part fixed. Importantly, because we wish to be able to modify the amount of the layer that is fixed during runtime, it is impossible to decompose this problem into two separate layers. Our implementation involves

5.2 Function Regression

Our first experiment is relatively simplistic, but is also indicative of the basic algorithm’s performance. In this experiment, we approximate the trigonometric sine function in the range of $[-2\pi, 2\pi]$. Our architecture for this experiment is extremely simple: it is merely a feedforward network with one hidden layer consisting of up to 500 nodes. This is sufficient capacity to learn the sine function with great accuracy, but can still be heavily affected by the training regime applied to it. We investigate the importance of the hidden layer’s capacity by testing static networks of 100 and 500 nodes, then comparing these results to a dynamically sizing network.

For this experiment, we split the network into quarters, and initialize them all before any training begins.

< Performance here has been very excellent overall. The results were in the presentation. >

5.3 MNIST Classifier

Modern deep learning algorithms have generally tended to be developed for image classification purposes, in part due to the original usage of convolutional neural networks. LeCun et al.’s original work with CNNs [17] was in designing a classifier for the MNIST dataset, a collection of monochrome handwritten digits

Tensorflow includes MNIST support as part of the base installation

< As above, this was in my presentation. Results were good, but not as improved as the previous example. Also, it’s important to note that small improvements to MNIST are pretty big because of high accuracy overall (99.32 vs 99.37 accuracy) >

5.4 CIFAR-100

One of the common modern image classification datasets is CIFAR-100, a set of 60000 images collected by researchers at the University of Toronto. It consists of 20 classes, each with 5 subclasses. For each of the 100 subclasses, there are 500 training images and 100 testing images. The images are in color, but are of low resolution at 32×32 ; the small size of the dataset makes it especially attractive as an experimental problem. Larger image classification datasets exist, such as the commonly used ImageNet, but due to its over 150GB download size and consequently longer training times, it was not considered for this thesis. Most modern deep learning papers include results on both CIFAR-10 (a smaller version of the same problem) and CIFAR-100; we choose CIFAR-100 as state of the art performance on CIFAR-10 is over 90%, leading to a closer and less separable grouping of experimental results. In doing this, we hope to avoid the problem seen on the MNIST problem, where it is extremely difficult to improve on results that are already nearly perfect.

A particular point of interest with CIFAR-100 is that there are relatively few images per class. This means that it is a dataset for which overfitting is a critical concern. Typical algorithms, without any specially designed methods, can often achieve around 60% accuracy on the testing dataset. This, however, tends to represent a hard limit, as training accuracy will usually hit nearly 100% accuracy. The difference between testing and training accuracy, especially with the limited data available, is the primary area of improvement for modern algorithms.

< CIFAR-100 is a dataset with 10 classes, each with 10 subclasses (e.g. jets, then different kinds of jets). Results are coming up very soon hopefully! >

5.5 Performance

We note that our algorithm involves nearly no overhead over the original architecture; a simple timing benchmark over 1000 epochs of MNIST indicates a performance difference of 3.5% (37.9 seconds versus 36.6 seconds), which is well within the margin of error. This is because all of the major time-consuming operations are performed on the GPU, to which our algorithm does not add significant stress.

Furthermore, by limiting the capacity of the network, we are able to achieve far faster initial training. The initial timing experiment was performed by applying the algorithm but forcing it to use the full capacity of the network initially; this is far from the original intent. By utilizing it in the same way as developed for the experiments, the first 1000 epochs of MNIST actually take 11.9 seconds. While the algorithm takes more epochs to converge, the increased speed of working through the initial epochs is a significant boon.

< Expanding on performance gains here because of the smaller trained network. Also, Tensorflow imposes some other interesting details here because of the array slicing necessary. >

Chapter 6

Discussion

< more to come as results become a little clearer, most of my time is going into CIFAR-100 experiments working >

6.1 Regularization

< talk about how fixing network capacity may act as a regularizer >

6.2 Generalization

< discuss how generalization was better with trained model >

Chapter 7

Conclusion

7.1 a brief summary of results

< what the section title says >

7.2 Future Work and Further Notes

< talk about shortcut connections, different trainable parameters, also extend literature to other directions of optimization >

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