Using Deep Learning for X-Ray Image Classification

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Declaration

This report has been prepared on the basis of my own work. Where other published and unpublished source materials have been used, these have been acknowledged.

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I would like to thank...

Abstract

ABSTRACT TBD

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1 Introduction

The aim of this project is to explore the use of Deep Learning in a practical situation. Deep Learning techniques have been used in a range of problems, such as image recognition [ref GoogleLeNet], natural language processing [ref Google Neural Machine Translation], playing games [ref AlphaGo] and self-driving cars [ref WayMo], among others. These techniques have often achieved cutting-edge performance on these tasks - for instance, surpassing human performance in the ImageNet task [ref ILSVRC], or beating the world champion Lee Sedol at the game Go [ref AlphaGo win]. As such, Deep Learning is an exciting branch of Machine Learning with the potential to make significant impacts in many areas of life. Indeed Deep Learning is one of (the?) largest areas of active research in Machine Learning at the time of writing [ref numbers of citations].

This project focuses on image recognition, as this is one of the areas where Deep Learning has seen its biggest successes. In particular, we will be applying Deep Learning to the MURA (**mu**sculoskeletal **ra**diographs) dataset, published by the Machine Learning Group at Stanford University [1]. This is a collection of 40,005 X-ray images of a part of the upper extremity - comprising the arm, shoulder, wrist, hand etc. Each image is from one of 14,656 studies of an individual patient, performed at a particular point in time on one of these parts of the upper extremity. Each study was labelled as normal or abnormal at the time of clinical interpretation by a radiologist from Stanford Hospital - and these labels have been published alongside the images themselves. Therefore the aim of this project is to use Deep Learning to perform binary image classification on this set of X-rays - classifying them as either normal or abnormal. This will be a supervised learning task, since we have clear labels for our data, and our aim is to predict them.

While any model developed as part of this project can only represent a toy solution to this problem, the principle of combining Deep Learning and medicine seems to be a good one. Inded this too is an area of active research, both within radiology [ref radiology], medical imaging [ref other DL/med image work] and medicine more widely [ref DL/med work]. The works cited of course represents only a small fraction of what is being done. Thinking optimistically, Deep Learning can help improve patient outcomes, produce results more quickly, alleviate pressure off medical pracitioners, reduce medical mistakes and improve medical decision-making. As such,

this represents good motivation for me to dip my toe into this area as part of my project.

2 Background

This section describes the background of Deep Learning, and the methodology behind the techniques used in this project.

2.1 Deep Learning

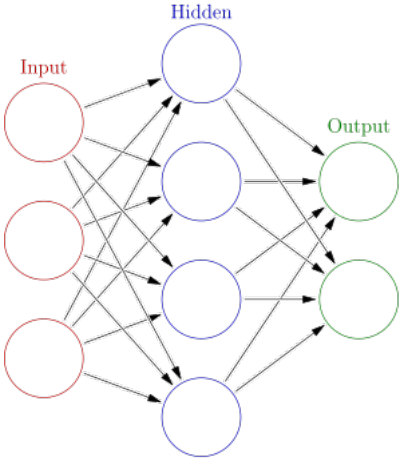
The main idea behind Deep Learning is for a system to learn representations of the data given to it. While these representations can start out simple, they are organised into a hierarchical sequence of layers so that simpler representations from earlier layers can be composed and built up into higher-level, more complex representations. This is repeated over many layers so that the final representations have sufficient information and detail for the task at hand. This process of building up complex representations from simpler parts means that feature engineering - the choice of which aspects of the data to include in the model, how they should be transformed or combined etc - is performed automatically by the system, as part of training. This is one of the great strengths of Deep Learning since feature engineering as a manual process can be difficult and time-consuming, especially when the data is very high-dimensional (as with images).

2.2 Artificial Neural Networks

2.2.1 Basic Structure

More specifically, these Deep Learning systems tend to be artificial neural networks (ANN's), of various forms depending on the nature of the task. A simple version of such a network [2] is shown in **Figure 1** below. These consist of a set of "neurons" (the circles in the image below) organised into layers, with each neuron from one layer connected to all neurons in the next layer. Each neuron has an associated activation, typically just a real number, which is derived from the activations of the neurons feeding into it from the previous layer. The input layer is a special case, where the neuron activations represent values from the item of data being fed into the network. For instance, for greyscale images, the input neurons correspond to each pixel in the given input image, and the input activations are simply each pixel's value. The activations of the final output layer may represent different things, depending on the task - for instance, the final learned representation of the data item when doing dimension reduction. Or, for classification, the probability distribution over the set of classes that captures the network's prediction of which class the given data item is in.

Figure 1: Example of a simple artificial neural network



The connections between the neurons from one layer to the next represent the network's weights, each weight again usually just a real number. In addition to these weights between layers, each neuron (aside from the input layer) has an associated bias, once again usually just a real number. Taken across the whole network, these weights and biases form the set of parameters that define the model. They dictate how the activations from neurons in the previous layer should be used to calculate the activations of neurons in the next layer. For instance, let the activations of the neurons in layer i be given by the vector $a^{[i]}$, and the weights connecting neurons in layer i to those in layer $i+1$ be given by the matrix $\mathbf{W^{[i+1]}}$. So if the numbers of neurons in layers i and $i+1$ respectively are n_i and n_{i+1}, then $a^{[i]}$ will have dimension $n_i \times 1$, and $\mathbf{W^{[i+1]}}$ dimension $n_i \times n_{i+1}$[1]. Then the activations for the neurons in layer $i+1$ are given by:

$$a^{[i+1]} = f_{i+1}(\mathbf{W^{[i+1]}}^\top a^{[i]} + b^{[i+1]})$$

where:

- $b^{[i+1]}$ is the vector of biases for the neurons in layer $i+1$ (so of dimension $n_{i+1} \times 1$).

[1]Each of the n_i neurons in layer i connects to each of the n_{i+1} neurons in layer $i+1$, making $n_i \times n_{i+1}$ connections in total.

- f_{i+1} is the activation function for layer $i+1$, that applies element-wise to the vector on which it operates, and hence returns a vector. The choice of activation functions is part of the design of the network.

This process is repeated, with activations from the input layer feeding into activations of the first hidden layer; activations from this hidden layer feeding into the next hidden layer; etc until the final activations in the output layer are produced. Note that while **Figure 1** above showed only one hidden layer between input and output, in practice there can be arbitrarily many hidden layers - each taking as input the activations from their previous layer, and sending their own activations as output to the next layer. The choice of the numbers of hidden layers, and the numbers of neurons in each of these layers is again part of the design of the network.

Such networks are called fully-connected networks, and theirs layers with every neuron connecting to every neuron in the next layer are called *fully-connected* or *dense* layers.

2.2.2 Activation Functions

The activation functions are usually chosen to be non-linear - since otherwise, composing several layers of neuron activations reduces to taking a linear function of the original input neurons and the network itself simply becomes a linear function. To see this, let $f(x) = x$ be the linear activation function used throughout the network. Then if layer 0 is the input layer, the activations of layer 1 are:

$$a^{[1]} = f(\mathbf{W^{[1]}}^\top a^{[0]} + b^{[1]}) = \mathbf{W^{[1]}}^\top a^{[0]} + b^{[1]}$$

And the activations for layer 2 are:

$$\begin{aligned} a^{[2]} &= f(\mathbf{W^{[2]}}^\top a^{[1]} + b^{[2]}) && (1)\\ &= \mathbf{W^{[2]}}^\top a^{[1]} + b^{[2]} && (2)\\ &= \mathbf{W^{[2]}}^\top (\mathbf{W^{[1]}}^\top a^{[0]} + b^{[1]}) + b^{[2]} && (3)\\ &= (\mathbf{W^{[1]}W^{[2]}})^\top a^{[0]} + \mathbf{W^{[2]}}^\top b^{[1]} + b^{[2]} && (4)\\ &= \mathbf{W'}^\top a^{[0]} + b' && (5) \end{aligned}$$

where:

- $\mathbf{W'} = \mathbf{W^{[1]}W^{[2]}}$ is an $n_0 \times n_2$ matrix

- $b' = \mathbf{W^{[2]}}^\top b^{[1]} + b^{[2]}$ is an $n_2 \times 1$ vector
- Equation (4) uses the matrix transpose rule $(AB)^\top = B^\top A^\top$

Hence both $a^{[1]}$ and $a^{[2]}$ are linear functions of $a^{[0]}$. This argument can be repeated to any number of hidden layers, and so the output of the whole network (regardless of its size) is simply a linear function of the input. This is undesirable since such a network cannot learn more complicated, non-linear features of the data. Training the network is effectively equivalent to just performing linear regression.

Therefore non-linear activation functions are usually preferred. In this project we have used the following activation functions, in line with standard practice for image classification [ref e.g. VGG16].

ReLU
The Rectified Linear Unit (ReLU) is a scalar activation function that takes a linear function of its argument above a certain threshold m, and is constant otherwise:

$$f(x) = max\{x, m\}$$

Note that m is a hyperparameter, specified in advance of training, rather than learning during it. Typically it is just set to 0 - as otherwise this implies some sort of prior knowledge about the scale of the "pre-activation" values $\mathbf{W^{[i+1]}}^\top a^{[i]} + b^{[i+1]}$ for all the various layers and neurons in the network (since m could theoretically be set on a neuron-by-neuron basis). This would be difficult to justify, especially when adjusting the level of these pre-activation values is already handled by the bias term $b^{[i+1]}$, a parameter that is learned during training.

This activation function introduces a non-linearity at the point $x = m$, since its slope jumps from 0 to 1 as x increases beyond m. While the function is linear above m, this non-linearity at m has proven sufficient in practice to obtain good results with ANN's.

Softmax
The Softmax can be regarded as a vector-to-vector function, that takes as input a vector v, of length (say) n, and produces an output vector w with the same length as v. The j^{th} component of w is given by:

$$w_j = f(v)_j = \frac{e^{v_j}}{\sum_{k=1}^{n} e^{v_k}}$$

where v_j is the j^{th} component of v. Since the Softmax involves exponentiation, it is clearly a non-linear function of its inputs, as desired. Now $e^x \geq 0 \ \forall \ x \in \mathbb{R}$, so we have $w_j \geq 0$. And, by definition:

$$\begin{aligned}\sum_{j=1}^{n} w_j &= \sum_{j=1}^{n} \frac{e^{v_j}}{\sum_{k=1}^{n} e^{v_k}} \\ &= \frac{\sum_{j=1}^{n} e^{v_j}}{\sum_{k=1}^{n} e^{v_k}} \\ &= 1\end{aligned}$$

Hence $w_j \in [0, 1] \ \forall \ j = 1, \ldots, n$ and so w represents a probability distribution over the set of values $1, \ldots, n$. This is true regardless of the scale or values of the input v.

This is extremely useful for classification, since we can set the final layer of our ANN to have the same number of neurons as numbers of classes, and let it use the Softmax activation function. Then each neuron would correspond to one of the w_j above, and the activations across the whole output layer would form a probability distribution over the set of classes. The network then provides a means to go from, say, an image to predicted probabilities of which class the image belongs to.

More concretely, for our purposes we set the final layer to have 2 neurons - corresponding to normal or abnormal respectively.

2.3 Training

After choosing the structure of the ANN - i.e. the numbers of layers, numbers of neurons, and activation functions for each layer/neuron - it remains to train the network. The act of training the network boils down to setting appropriate values for all the weights and biases across the whole network. While this could be done by hand - this would be very difficult and, for larger networks, the numbers of weights and biases can be several million and hence infeasible to set by hand anyway. Instead, the weights[2] are initialised to random values and then automatically updated through a process called *Backpropagation*. This involves the following steps:

- **Forward Pass:** data items are input into the network (via the input layer). The activations of each of the subsequent layers are then calculated based on this input, up to the final output layer. Then (since our problem is supervised learning) the output is compared to known, true label for the given data item. This comparison is quantified by a loss function, some chosen function that measures how close the prediction is to the true label.

- **Backward Pass:** Since the value of the loss function depends on the network's weights (via the predicted label), the gradient of the loss function with respect to each of the weights can be calculated. These gradients then tell us how to adjust (in what direction, by how much) each of the weights in order to reduce the loss - and hence make the prediction closer to the true label.

- **Weight Update:** It remains to make these changes to the weights. Typically we only make a small change vs that indicated by the gradient - since the gradients themselves will be subject to a lot of random variation from data item-to-data item. So making the full change will result in noisy, erratic weight changes, and hence also erratic changes in the predictions with each weight update. So instead we multiply all of the gradients by some small number η (e.g. $\eta \approx 0.001$) called the *learning rate*. This has the effect of slowing down the weight updates, and hence allowing a more gradual progression towards a minimum of the loss function.

There are in fact a number of different training algorithms, which vary in the details, but all of the ones we consider follow this basic pattern.

[2] We'll use "weights" as a shorthand for "weights and biases" - i.e. the set of model parameters - except where a distinction between the two is necessary.

2.3.1 Loss Functions

As mentioned, loss functions are used to measure how far away predicted labels, generated by the network, are from the true label. Predictions that are "close" to the true label should have a smaller loss than predictions that are further away. For any item of data, both the activations in the network's input layer, and the item's true label are fixed. So the only aspect of a given network that we are free to vary are its weights, since these determine how the prediction is generated for an item of data. Therefore we can regard the loss as a function of the network's weights - and the goal of training is to set these weights so as to minimise the expected loss over a collection of data items.

The loss function we have used in this project is the cross-entropy loss, again in line with standard practice for image classification.

Cross-Entropy Loss
The cross-entropy loss assumes that the true label y (i.e. the class to which the data item belongs) is coded as a "one-hot" vector. If there are n classes, y is a vector of length n, with each component corresponding to one of these classes. All components of y are set to 0, except for the component corresponding the class to which y belongs - which is set to 1.

So for our x-ray data we code the two classes as follows:

- Normal: $[1, 0]$
- Abnormal: $[0, 1]$

The predicted label $\hat{y}$, per the Softmax activation function in the output layer, represents a probability distribution over the n classes - and so has the same dimension as y.

The cross-entropy loss is then given by:

$$L(y, \hat{y}) = -\sum_{j=1}^{n} y_j log(\hat{y_j})$$

Note that since y has all components 0, except for a 1 corresponding to the true label, the loss above reduces to taking the logarithm of the predicted probability of the true label. The sign of the logarithm is negated, so that smaller probabilties, which would give larger negative values of log, give

larger positive loss values. The loss is therefore monotonically decreasing with the predicted probability of the true label - which is as desired, since predicting a high probability for the true label should have a smaller loss than predicting a lower probability.

2.3.2 Backward Pass

After performaing a forward pass and calculating the loss for a given data item, we now calculate the gradients of the loss with respect to all the weights and activations in the network. This is called a backward pass since the gradients in one layer depend on those in the subsequent layer. Hence the process starts with calculating gradients in the output layer, then the gradients for the previous layer, and so on all the way back through the whole network. While the weight update step of the Backpropagation algorithm only uses the gradients of the weights, these gradients themselves depend on the gradients of the activations of the neurons which depend on these weights. Thus the backward pass involves calculating the gradients of activations, even though these are not strictly used in the weight update step.

Using the cross-entropy loss function, for a classification task as described above, we can calculate the gradient of the loss with respect to $\hat{y_j}$ (considering y_j as a fixed constant):

$$\begin{aligned}\frac{\partial L}{\partial \hat{y_j}} &= \frac{\partial}{\partial \hat{y_j}}(-\sum_{j=1}^{n} y_j log(\hat{y_j})) \\ &= \frac{\partial}{\partial \hat{y_j}}(-y_j log(\hat{y_j})) \\ &= -\frac{y_j}{\hat{y_j}}\end{aligned}$$

Recall that $\hat{y_j}$ is the activation of the j^{th} neuron in the output layer. Which itself is a derived from the weights $\mathbf{W}$ and biases b in the output layer, and the activations from the previous layer (layer l, say) $a^{[l]}$, fed through the Softmax function:

$$\begin{aligned}z &= \mathbf{W}^\top a^{[l]} + b \\ \hat{y_j} &= \frac{e^{z_j}}{\sum_{k=1}^{n} e^{z_k}}\end{aligned}$$

And so, by the quotient rule:

$$\begin{aligned}\frac{\partial \hat{y}_j}{\partial z_j} &= \frac{e^{z_j}(\sum_{k\neq j} e^{z_k} + e^{z_j}) - (e^{z_j})^2}{(\sum_{k=1}^{n} e^{z_k})^2} \\ &= \frac{e^{z_j}}{\sum_{k=1}^{n} e^{z_k}} \frac{\sum_{k\neq j} e^{z_k}}{\sum_{k=1}^{n} e^{z_k}} \\ &= \hat{y}_j(1-\hat{y}_j)\end{aligned}$$

Where the final equality is due to:

$$\begin{aligned}1 - \hat{y}_j &= 1 - \frac{e^{z_j}}{\sum_{k=1}^{n} e^{z_k}} \\ &= \frac{\sum_{k=1}^{n} e^{z_k} - e^{z_j}}{\sum_{k=1}^{n} e^{z_k}} \\ &= \frac{\sum_{k\neq j} e^{z_k}}{\sum_{k=1}^{n} e^{z_k}}\end{aligned}$$

Therefore we can apply the chain rule of differentiation to calculate the gradients of the loss with respect to the weights and biases in the output layer as follows:

$$\begin{aligned}\frac{\partial L}{\partial z_j} &= \frac{\partial L}{\partial \hat{y}_j}\frac{\partial \hat{y}_j}{\partial z_j} \\ &= \frac{y_j}{\hat{y}_j}\hat{y}_j(1-\hat{y}_j) \\ &= y_j(1-\hat{y}_j)\end{aligned}$$

Now if layer l has n_l neurons[3]:

$$z_j = \sum_{i=1}^{n_l} w_{i,j} a_i^{[l]} + b_j$$

So:

$$\frac{\partial z_j}{\partial w_{i,j}} = a_i^{[l]}$$

$$\frac{\partial z_j}{\partial b_j} = 1$$

[3]Technically since we are using the Softmax activation function in the output layer, n_l must match the number of neurons in the output layer, n.

And we have:

$$\begin{aligned}\frac{\partial L}{\partial w_{i,j}} &= \frac{\partial L}{\partial z_j}\frac{\partial z_j}{\partial w_{i,j}} \\ &= y_j(1-\hat{y_j})a_i^{[l]}\end{aligned}$$

$$\begin{aligned}\frac{\partial L}{\partial b_j} &= \frac{\partial L}{\partial z_j}\frac{\partial z_j}{\partial b_j} \\ &= y_j(1-\hat{y_j})\end{aligned}$$

where $w_{i,j}$ is an element from j^{th} column of the weight matrix $\mathbf{W}$, and b_j the bias of the j^{th} neuron in the output layer.

We can also obtain similar formulas for the gradients of the loss with respect to the activations in layer l. Since each neuron in this layer connects to all neurons in the output layer, a given activation $a_i^{[l]}$ will appear in the formula (as shown above) for all z_j, $j = 1, \ldots, n$. And each of the z_j appear additively in the loss function via $\hat{y_j}$. Therefore we have:

$$\frac{\partial z_j}{\partial a_i^{[l]}} = w_{i,j}$$

$$\begin{aligned}\frac{\partial L}{\partial a_i^{[l]}} &= \sum_{j=1}^{n}\frac{\partial L}{\partial z_j}\frac{\partial z_j}{\partial a_i^{[l]}} \\ &= \sum_{j=1}^{n} y_j(1-\hat{y_j})w_{i,j}\end{aligned}$$

But these activations $a^{[l]}$ themselves depend on the weights and biases in layer l, and so we can extend the chain rule further to calculate the gradient of the loss with respect to these as well. And we can repeat this process for the activations, weights and biases, in layers $l-1, l-2, \ldots$ etc all the way back through the entire network.

2.3.3 Weight Update

The gradients calculated in the backward pass above give the change in weight to make, in order to increase the loss function. Since we aim to decrease our loss function, we subtract the gradients from the current values

of all the weights. However, as mentioned, we first multiply the gradients by a hyperparameter η, called the learning rate, in order to avoid large, erratic changes in weights (and hence predictions) after each weight update. That is, for a weight (or bias) w in the network, with gradient $\frac{\partial L}{\partial w}$ we apply the following update:

$$w = w - \eta \frac{\partial L}{\partial w}$$

2.3.4 Optimisers

The following algorithms are all variations on the general theme of Back-propagation described above. That is, they all concern how to set the weights in order to minimise the loss function, based on the gradients of the loss function (hence the algorithms are called "optimisers").

Gradient Descent
This involves performing a forward pass, calculating the activations and the loss, then performing a backward pass, calculating the gradients of all the weights, for every item of data in the training set. The gradients of each weight are then averaged across the entire set of training data, before performing the weight update using these average values for each weight. That is, for a weight w let $\frac{\partial L}{\partial w_i}$ be its gradient after forward and backward passes with the i^{th} element of the training set as input to the network. Then if there are n items of data in the training set, perform the following weight update:

$$w = w - \frac{\eta}{n} \sum_{i=1}^{n} \frac{\partial L}{\partial w_i}$$

That is, we have to perform a forward pass and backward pass for every item in the training set, and keep track of all associated gradients, before making a single weight update. This can be both slow and consume a lot of memory (consider a large network with millions of weights, and a large training set with millions of items). Note this process will often be repeated, with training involving hundreds or thousands of weight updates.

Stochastic Gradient Descent
Stochastic gradient descent (SGD) aims to speed things up by dividing the training set up into batches of a certain size (say, 128). Each data item in the training set is assigned randomly (hence "stochastic") without replacement to each of the batches. Then the weight updates are performed

after calculating and averaging the gradients for each item in a batch. That is, if the batches are of size m, for a given weight we make the following update:

$$w = w - \frac{\eta}{m} \sum_{i=1}^{m} \frac{\partial L}{\partial w_i}$$

where $\frac{\partial L}{\partial w_i}$ is the gradient of w for the i^{th} item in the batch. An *epoch* is then defined as a pass through the full set of batches, performing a weight update for each batch. Thus if the training data of size n is split up into batches of size m, an epoch would involve $\left\lceil \frac{n}{m} \right\rceil$[4] weight updates - compared to just one for ordinary Gradient Descent. Training using SGD often involves running for several epochs. The random assignment of the training data into batches is repeated fresh at the start of each epoch.

The advantage of SGD is that it is clearly quicker than GD to perform weight updates. While each weight update will be subject to more randomness than in GD, since each update corresponds to a single, random batch rather than the full training set. However, over the course of several hundred or thousand weight updates, involving many epochs or passes over the whole training set, this should average out to give comparable results to GD.

RMSProp

One of the issues with GD and SGD is that the learning rate η is a global hyperparameter that is fixed for all the weights in the network, and for all weight update iterations. However in practice, some weights in the network will require larger or smaller updates than others and, over the course of training, the weight updates will usually need to get smaller and smaller for successive iterations, as we approach a minimum of the loss function. RMSProp aims to solve these problems by effectively allowing the learning rate to vary during training and for each weight.

Let w_t be a weight in the network, and let $g_t = \frac{\partial L}{\partial w_t}$ be its gradient, at iteration t. Then over all iterations we keep an exponential moving average of the square of these gradients:

$$v_t = \alpha g_t^2 + (1 - \alpha) v_{t-1}$$

[4] $\lceil x \rceil$ is the smallest integer greater than or equal to x. If m does not divide into n, the final batch will comprise ($n \mod m$) items to ensure an epoch covers the entire training set.

where the base case is $v_0 = 0$, and $\alpha \in [0, 1]$ is a chosen hyperparameter that determines the extent to which (squared) gradients from past iterations affect the value of v_{t+1}. Note that an iteration can refer either to a full pass over the whole training set, as in GD, or over a batch, as in SGD. Although in practice we will use it in conjunction with SGD, since it inherits the benefits mentioned above. So the "gradient" g_t above would in fact be the average of the gradients for the weight across a batch. The weight update for the given iteration is then:

$$\delta_t = \frac{\eta}{\sqrt{v_t} + \epsilon} g_t$$

$$w_{t+1} = w_t - \delta_t$$

where η is the (global) learning rate, and ϵ is some small number (e.g. $\epsilon = 10^{-6}$) added to avoid division by 0. The $\frac{\eta}{\sqrt{v_t} + \epsilon}$ term now means that the learning rate η is dampened by the factor $\sqrt{v_t} + \epsilon$, which varies for each training iteration and for each weight in the network. So for a weight that had larger gradients in previous iterations, so a larger v_t, the effective learning rate will be smaller. Hence its subsequent weight updates get smaller as training progresses - slowing them down compared to weights with smaller gradients and weight updates at earlier iterations. This is desired, since weights that have seen large changes over training are more likely to be closer to the loss function minimum on which they are converging, and so should progress more slowly towards it (to avoid overshooting it, or other erratic behaviour).

Adam

The Adam ("Adaptive Momentum") optimiser is a variation on RMSProp that takes account of momentum in the gradients from previous epochs. That is, large gradients on several previous iterations should not be ignored if the current gradient (by chance) happens to be very low, or vice versa. The momentum effect produces smoother and less erratic weight updates than RMSProp. To this end, Adam maintains an exponential moving average of the gradient g_t, as well as the squared gradient of RMSProp:

$$m_t = \beta g_t + (1 - \beta) m_{t-1}$$

Again the base case is $m_0 = 0$, and $\beta \in [0, 1]$ is another hyperparameter that determines to what extent past gradients are taken credit for. The weight update is then:

$$\delta_t = \frac{\eta}{\sqrt{v_t} + \epsilon} m_t$$

$$w_{t+1} = w_t - \delta_t$$

where v_t, η and ϵ are defined as in RMSProp. This has the same benefits as RMSProp of dampening the learning rate η during training, but the weight update uses the smoothed m_t rather than the raw g_t at each iteration.

2.3.5 Weight Initialisation

Prior to training, all weights and biases in the network need to be initialised to some reasonable values. If they were all simply set to 0, the activations of all neurons in the network, and hence all the gradients would just be 0 too. Therefore the weight update step would leave all weights unchanged, and "training" would accomplish nothing. Instead weights are usually initialised to random values. This effectively sets the initial position on the (multidimensional) loss surface, considering the loss as a function of the network's weights. Training then proceeds from this initial position towards a minimum of this loss function. Therefore performing different instances of training (even on the same data) ab-initio can lead to different solutions, since each instance will have a different starting position on the loss surface, and hence converge toward different minima. However the choice of optimiser should help mitigate this problem, e.g. by avoiding shallow local minima, and progressing towards deeper, more global minima[5]. For this project we have used the following weight initialisation scheme, since that is the default in the software (Keras) we used to train our models.

Glorot Uniform

This initialisation scheme was introduced by Xavier Glorot and Yoshua Bengio in 2010 [3]. It initialises biases to 0, and the weights $w_{i,j}$ in each layer randomly according to the distribution:

$$w_{i,j} \sim U[-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}]$$

where $U[a, b]$ is the continuous random uniform distribution over the interval $[a, b]$, and n is the number of neurons in the previous layer.

[5]Of course, the loss surface is usually very high dimensional, and depends on the training data. So it is hard to have any clarity over its precise form or nature. In any case, it is often not necessary for the task at hand - networks are typically trained until they achieve some desired level of performance, regardless of whether this represents a true global minimum or not.

In fact, examining the Keras source code [4], Glorot Uniform is implemented slightly differently to how it was introduced by Glorot & Bengio. Biases are still initialised to 0. However weights are drawn randomly from $U[-limit, limit]$ with $limit = \sqrt{\frac{6}{fan\_in + fan\_out}}$ where fan_in is the number of input neurons to the weight tensor, and fan_out the number of output neurons. In our terms, if $\mathbf{W}$ is the $n_i \times n_{i+1}$ matrix of weights connecting layers i and $i+1$, then each element w of $\mathbf{W}$ will be initialised as above, with $fan\_in = n_i$ and $fan\_out = n_{i+1}$.

2.4 Convolutional Neural Networks

Convolutional neural networks (CNN's) are a variant of artificial neuron networks described above, that are often used for image processing tasks such as classification. They are organised as a sequence of "convolution" layers, where the first layer operates directly on an image to produce a representation of it comprised of various low-level features, such as edges or patches of light or dark etc. The next layer then operates on this representation, producing another representation that captures slightly higher-level features, based on compostions of the low-level features from the first layer. This process is repeated for a chosen number of layers, with each layer outputting a representation based on the one from the previous layer. The final output from the sequence of convolution layers is then some representation of the original image built up from the low- and mid-level features from past layers. This final representation can then be used for the task at hand - for instance fed through a fully-connected layer, into a Softmax output layer for classification.

The strength of CNN's is that the representations they produce can pick up features regardless of where they appear in the image. So if a representation captures the shape and colour of eyes (say), it will "recognise" eyes that appear at any position in the image. This property is called *translational invariance*. By contrast, if the original image was fed through a sequence of fully-connected layers, different weights in the network would correspond to different positions in the image. So that any feature learned by some subset of the weights would only be recognised if it appeared at the corresponding position in the image.

Another strength is that the numbers of weights in convolution layers are not tied to the size of the image, whereas a fully-connected layer would be. Therefore the number of weights in a given layer can be significantly smaller than for a corresponding fully-connected layer. This makes training the network easier, since there are fewer weights to set. For instance, consider a 100×100 image fully-connected to a hidden layer of 10 neurons - this would have $100 \times 100 \times 10 = 100,000$ weights. Meanwhile a convolution layer might have, say, 30 3×3 filters - making $30 \times 3 \times 3 = 270$ weights. This independence from the size of images means that previously-trained CNN's can be used on different sets of images (potentially of entirely different dimensions) from those it was originally trained on, and still identify the same features in both sets of images. This makes CNN's very convenient

for transferring from one image processing task to another.

2.4.1 Image Representation

Throughout this section, we represent an image as either a 2D or 3D grid of pixel values, where the height and width of the image are the first two dimensions, and the channels of the image are the third dimesion. For greyscale images, there is only one channel, so we regard the image as being 2D. For colour images coded as RGB (say), there are three channels (red, green, blue) so we regard the image as 3D with depth 3.

2.4.2 Convolution Layers

A convolution layer represents a collection of *filters* of a chosen dimension - say, 3×3. Each element of a filter is a real number, and is one of the weights of the convolution layer to be learned during training. In fact a filter will operate on all channels of its input image or representation (from previous convolution layers). So a 3×3 filter working on an RGB image will have $3 \times 3 \times 3 = 27$ weights, since the image has 3 channels. The output of each filter in a convolution layer is passed to the next convolution layer as a separate channels - so that if the first layers has (say) 32 filters, the filters in the next layer will have a depth of 32. That is if the next layer uses 5×5 filters, each one will have $5 \times 5 \times 32 = 800$ weights[6].

Each filter performs a convolution operation between its input and its weights. For a one-channel input, this is defined as follows. Let $\begin{bmatrix} w_{1,1} & w_{1,2} \\ w_{2,1} & w_{2,2} \end{bmatrix}$ be a 2×2 filter and b be its associated bias. Let $\begin{bmatrix} p_{1,1} & p_{1,2} \\ p_{2,1} & p_{2,2} \end{bmatrix}$ be the values for some contiguous 2×2 region of the input. The convolution is then:

$$z = \sum_{i=1}^{2} \sum_{j=1}^{2} w_{i,j} p_{i,j} + b$$

$$a = f(z)$$

where f is some chosen activation function (e.g. ReLU). For a multiple-channel input, the filter and input will be 3-dimensional, and the opertation

[6] In fact, each filter has a single associated bias term (regardless of depth), so the filters mentioned would have 28 and 801 parameters respectively.

would instead apply to a contiguous 3D volume of the input. For instance, if the input were an RBG image, the convolution would look like:

$$z = \sum_{i=1}^{2} \sum_{j=1}^{2} \sum_{k=1}^{3} w_{i,j,k} p_{i,j,k} + b$$

This convolution operation is repeated multiple times, at each possible position in the input.

2.4.3 Padding

2.4.4 Pooling Layers

2.5 Prediction

Write about generating predictions from the networks

2.6 Performance Measures

Write about performance measures - ROC curve, Cohen's Kappa etc Discuss train vs valid performance, overfitting etc.

2.7 State-of-the-Art

What is the current image processing SOTA - e.g. ILSVRC Anything done specifically for radiology?

2.8 Pretrained Models

Discuss the use of pre-trained models - can keep weights the same, replact the head. Describe the structure of the pre-trained models we'll use for comparison: [MAYBE PUT INTO APPENDIX?]

2.8.1 VGG16

Describe VGG16

3 Data

Write about the MURA data, show some exmaple images (normal & abnormal), give data breakdowns

3.1 MURA

Discuss MURA - what it is, how it was produced

3.2 Image Examples

As can be seen in **Figure 2** below, the x-ray is of a hand. A side-profile of the hand from the same study can be seen in **Figure 3**. **Figure 4** is a copy of **Figure 3**.

Figure 2: Example X-Ray Image

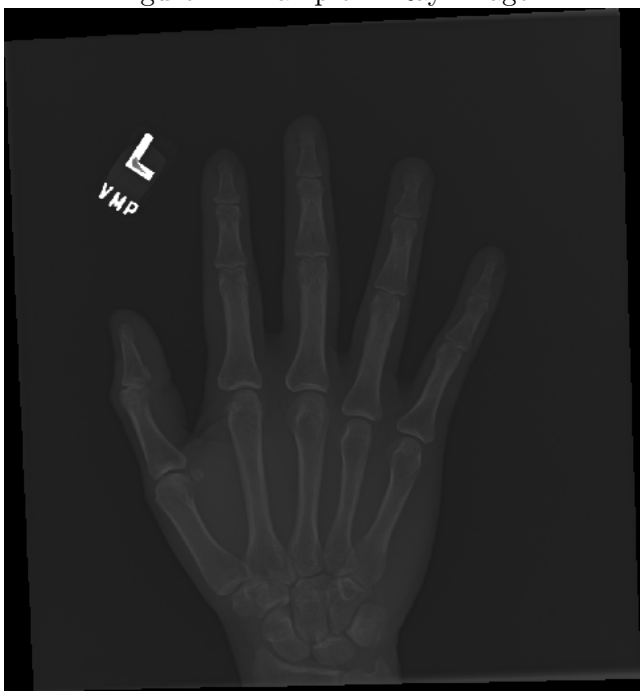


Figure 3: Another example X-Ray Image

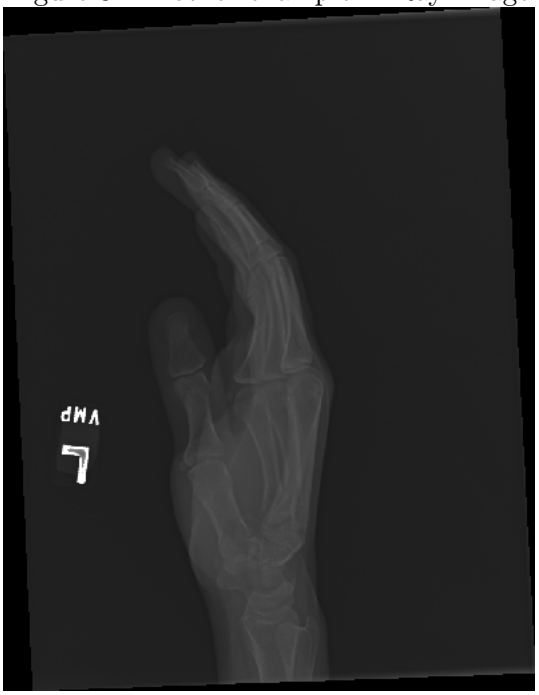
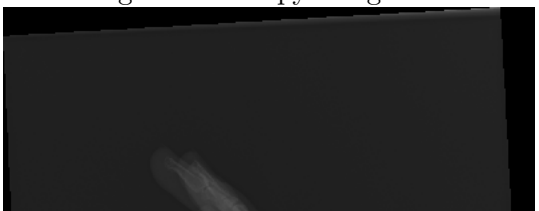


Figure 4: A copy of figure 2



3.3 Data Breakdowns

Data breakdowns

4 Model Development

4.1 Working Environment

Describe google cloud set-up, GPU, python packages used etc

4.2 Data Preprocessing

Describe the preprocessing work done on the data - resize images, normalise values, data augmentation etc

4.3 Model

Describe the final ab-initio model I end up with - structure, loss function, training params/hyperparams etc

4.4 Predictions

Discuss getting predictions and aggregating down to study-level predctions

5 Results

5.1 Baseline Performance

Give the performance of my chosen ab-initio model

5.2 Image Size

How do my results vary with size of image? Does increasing image size increase scope for

5.3 Regularisation

Perform some regularisation experiments, show results

5.4 Pre-Trained Models

How does my model compare vs a selection of pretrained models

6 Conclusions

Include introspective chapter Work here not comparable to clinical setting, e.g. smaller, lower resoution images; radiologist may have a relationship with patient - know medical history, other symptoms etc What is "abnormal"? - type & severity of abnormality not known, MURA paper not clear.

7 Professional and Ethical Issues

Potential Impact on Radiology - Deep Learning tools used to help triage/prioritise radiologists' work, not replace them; Can we trust diagnosis to a computer program? Would you be happy to do so? Conversely - medical errors happen a lot (est. cost $X p.a.; any specifics for radiology?) but DL tools may at least help cut that down.

8 Extensions

Enquire further about what "abnormal" means Alternative data e.g. CheXNet, others(?) Alter NN to accept multiple images simultaneously and so predict based on several views at once (e.g. by weight-sharing, or appening all study images into a single 3D tensor)

References

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[2] "Artificial neural network." `https://en.wikipedia.org/wiki/Artificial_neural_network`, 2018. [Online; accessed 5-August-2018].

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A Pretrained Model Architechtures

Below we describe the architechtures of the various pre-trained neural network models mentioned in the text.

A.1 VGG16

This is the VGG16 model.