Abstract

Machine learning is a growing area in computer science. Neural networks is very popular subdomain of it. This project generally covers the work of M. Nielsen and his book Neural Networks and Deep Learning[1]. We will first introduce neual networks and then aplly it to a generic problem which is called classifying handwritten digits.

1. Introduction

The idea of neural networks is to take a large number of dataset known as training examples, and then develop a system which can learn from those training examples. In other words, the neural network uses the examples to automatically infer rules for recognizing other unknown examples. Furthermore, by increasing the number of training examples, the network can learn more about handwriting, and so improve its accuracy.

There are just 100 training digits below, perhaps we could build a better handwriting recognizer by using thousands or even millions or billions of training examples.

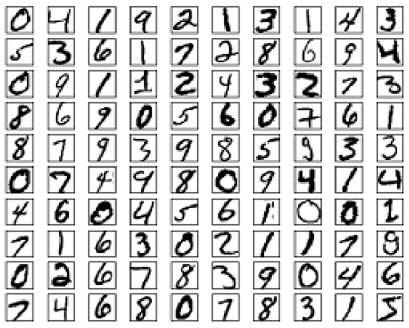


Figure 1: 100 Handwritten Digits

This project is concerned with write a computer program implementing a neural network that learns to recognize handwritten digits.

Along the way there are many key ideas about neural networks, including two important types of artificial neuron (the perceptron and the sigmoid neuron), and the standard learning algorithm for neural networks, known as stochastic gradient descent.

1.1. Perceptrons

Perceptron is a type of artificial neuron. Perceptrons were developed in the 1950s and 1960s by the scientist Frank Rosenblatt, inspired by earlier work by Warren McCulloch and Walter Pitts. Today, it's more common to use other models of artificial neurons - in this book, and in much modern work on neural networks, the main neuron model used is one called the sigmoid neuron.

A perceptron takes several binary inputs, $x_1, x_2, \ldots$, and produces a single binary output:

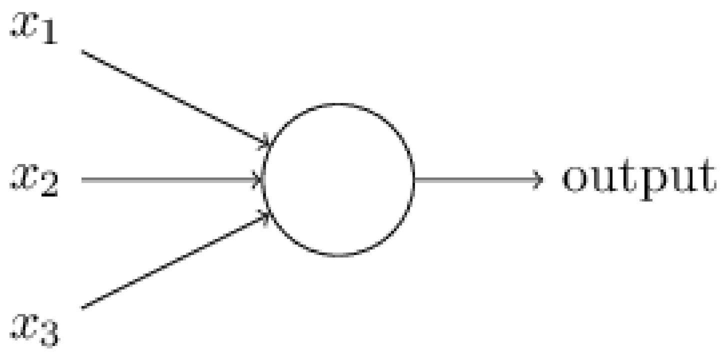


Figure 2: Perceptron

In general it could have more or fewer inputs. Rosenblatt proposed a simple rule to compute the output. He introduced weights, $w_1, w_2, \ldots$, real numbers expressing the importance of the respective inputs to the output. The neuron's output, 0 or 1, is determined by whether the weighted sum $\sum_j w_j x_j$ is less than or greater than some threshold value. Just like the weights, the threshold is a real number which is a parameter of the neuron. To put it in more precise algebraic terms:

$$output = \begin{cases} 0, & if \quad \sum_j w_j x_j \leqslant threshold \\ 1, & if \quad \sum_j w_j x_j > threshold \end{cases} \tag{1}$$

That's all there is to how a perceptron works!

That's the basic mathematical model. A way you can think about the perceptron is that it's a device that makes decisions by weighing up evidence.

Obviously, the perceptron isn't a complete model of human decision-making! But what the example illustrates is how a perceptron can weigh up different kinds of evidence in order to make decisions. And it should seem plausible that a complex network of perceptrons could make quite subtle decisions:

In this network, the first column of perceptrons - the first layer of perceptrons - is making three very simple decisions, by weighing the input evidence. What about the perceptrons in the second layer? Each of those perceptrons is making a decision by weighing up the results from the first layer of decision-making. In this way a perceptron in the second layer can make a decision at a more complex and more abstract level than perceptrons in the first layer. And even more complex decisions can be made by the perceptron in the third layer. In this way, a many-layer network of perceptrons can engage in sophisticated decision making.

In the first example, it is defined perceptrons has just a single output. In the network above the perceptrons look like they have multiple outputs. In fact, they're still single output. The multiple output arrows are merely a useful way of indicating that the output from a perceptron is being used as the input to several

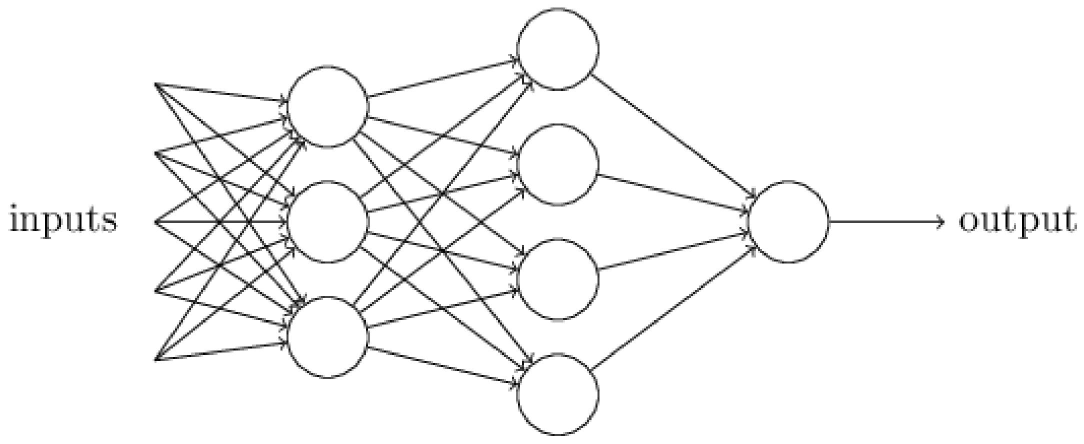


Figure 3: Multilayer Perceptron (MLP)

other perceptrons. It's less unwieldy than drawing a single output line which then splits.

Let's simplify the way we describe perceptrons. The first change is to write $\sum_j w_j x_j$ as a dot product, $w \cdot x \equiv \sum_j w_j x_j$, where w and x are vectors whose components are the weights and inputs, respectively. The second change is to move the threshold to the other side of the inequality, and to replace it by what's known as the perceptron's bias, $b \equiv$ *threshold*. Using the bias instead of the threshold, the perceptron rule can be rewritten:

$$output = \begin{cases} 0, & if \quad w \cdot x + b \leq 0 \\ 1, & if \quad w \cdot x + b > 0 \end{cases} \tag{2}$$

You can think of the bias as a measure of how easy it is to get the perceptron to output a 1. Or to put it in more biological terms, the bias is a measure of how easy it is to get the perceptron to fire. For a perceptron with a really big bias, it's extremely easy for the perceptron to output a 1. But if the bias is very negative, then it's difficult for the perceptron to output a 1.

1.2. Sigmoid neurons

Suppose we have a network of perceptrons that we'd like to use to learn to solve some problem. For example, the inputs to the network might be the raw pixel data from a scanned, handwritten image of a digit. And we'd like the network to learn weights and biases so that the output from the network correctly classifies the digit. To see how learning might work, suppose we make a small change in some weight (or bias) in the network. What we'd like is for this small change in weight to cause only a small corresponding change in the output from the network. As we'll see in a moment, this property will make learning possible. Schematically, here's what we want (obviously this network is too simple to do handwriting recognition!):

If it were true that a small change in a weight (or bias) causes only a small change in output, then we could use this fact to modify the weights and biases to get our

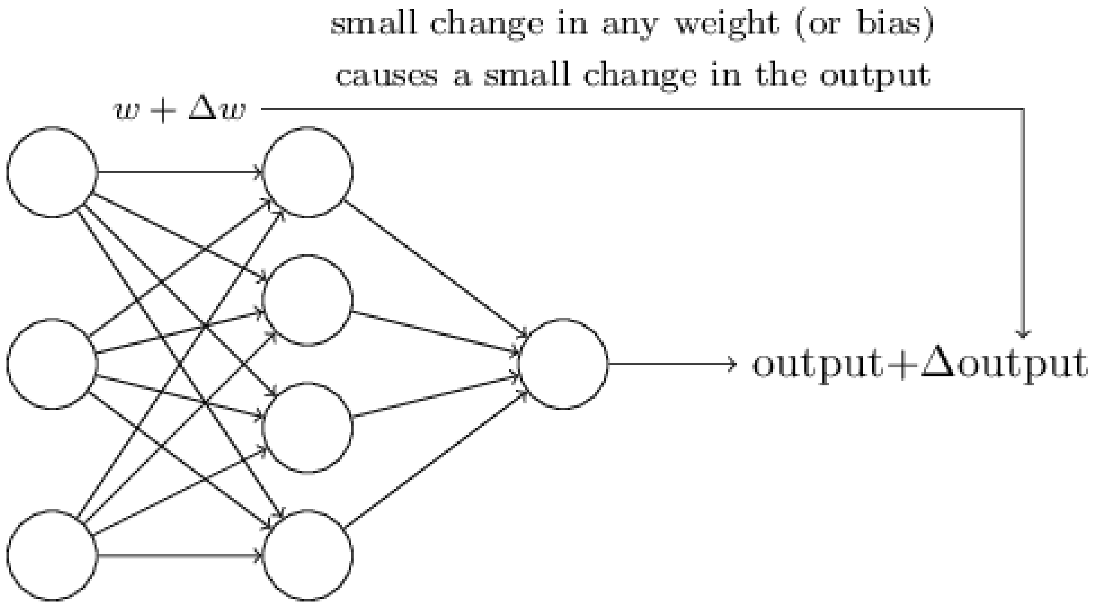

small change in any weight (or bias)
causes a small change in the output
$w + \Delta w$
output+Δoutput

Figure 4: Effects of changing weights to the output

network to behave more in the manner we want.

The problem is that this isn't what happens when our network contains perceptrons. In fact, a small change in the weights or bias of any single perceptron in the network can sometimes cause the output of that perceptron to completely flip, say from 0 to 1. That flip may then cause the behaviour of the rest of the network to completely change in some very complicated way.

We can overcome this problem by introducing a new type of artificial neuron called a sigmoid neuron. Sigmoid neurons are similar to perceptrons, but modified so that small changes in their weights and bias cause only a small change in their output. That's the crucial fact which will allow a network of sigmoid neurons to learn.

Okay, let me describe the sigmoid neuron. We'll depict sigmoid neurons in the same way we depicted perceptrons. Just like a perceptron, the sigmoid neuron has inputs, $x_1, x_2, \ldots$ But instead of being just 0 or 1, these inputs can also take on any values between 0 and 1. So, for instance, 0.638 is a valid input for a sigmoid neuron. Also just like a perceptron, the sigmoid neuron has weights for each input, $w_1, w_2, \ldots$ and an overall bias, b. But the output is not 0 or 1. Instead, it's $\sigma(w \cdot x + b)$, where σ is called the sigmoid function - sometimes called logistic function - and this new class of neurons called sigmoid neurons or logistic neurons. and is defined by:

$$\sigma(z) \equiv \frac{1}{1 + e^{-z}} \tag{3}$$

The output of a sigmoid neuron with inputs $x_1, x_2, \ldots$ weights $w_1, w_2, \ldots$ and bias b is

$$\frac{1}{1 + exp(\sum_j w_j x_j b)} \tag{4}$$

To understand the similarity to the perceptron model, suppose $z \equiv w \cdot x + b$ is a large positive number. Then $e^z \approx 0$ and so $\sigma(z) \approx 1$ just as it would have been for a perceptron. Suppose on the other hand that $z = w \cdot x + b$ is very negative. Then $e^z \to \infty$, and $\sigma(z) \approx 0$ like a perceptron. The shape is:

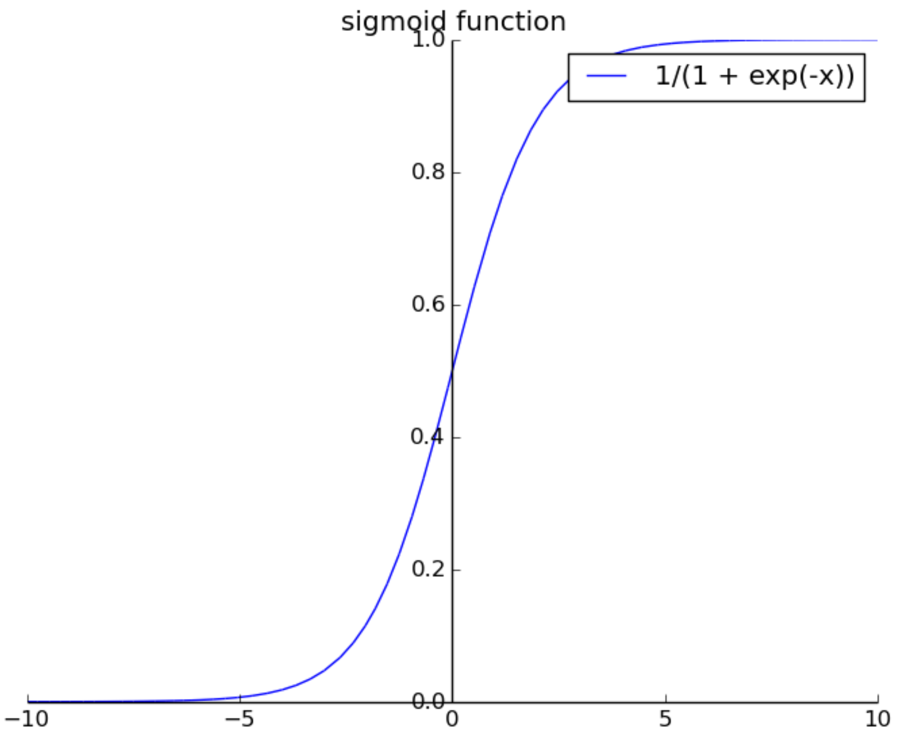


Figure 5: Sigmoid function

This shape is a smoothed out version of a step function or Heaviside step function:

If σ had in fact been a step function, then the sigmoid neuron would be a perceptron, since the output would be 1 or 0 depending on whether $w \cdot x + b$ was positive or negative. Actually, when $w \cdot x + b = 0$ the perceptron outputs 0, while the step function outputs 1. So, strictly speaking, we would need to modify the step function at that one point.

By using the actual σ function we get, a smoothed out perceptron. The smoothness of σ means that small changes Δw_j in the weights and Δb in the bias will produce a small change $\Delta output$ in the output from the neuron. In fact, calculus tells us that $\Delta output$ is well approximated by

$$\Delta output \approx \sum_j \frac{\partial\ output}{\partial w_j} \Delta w_j + \frac{\partial\ output}{\partial b} \Delta b \tag{5}$$

where the sum is over all the weights, w_j, and $\frac{\partial\ output}{\partial w_j}$ and $\frac{\partial\ output}{\partial b}$ denote partial derivatives of the output with respect to w_j and b, respectively. So while sigmoid neurons have much of the same qualitative behaviour as perceptrons, they make

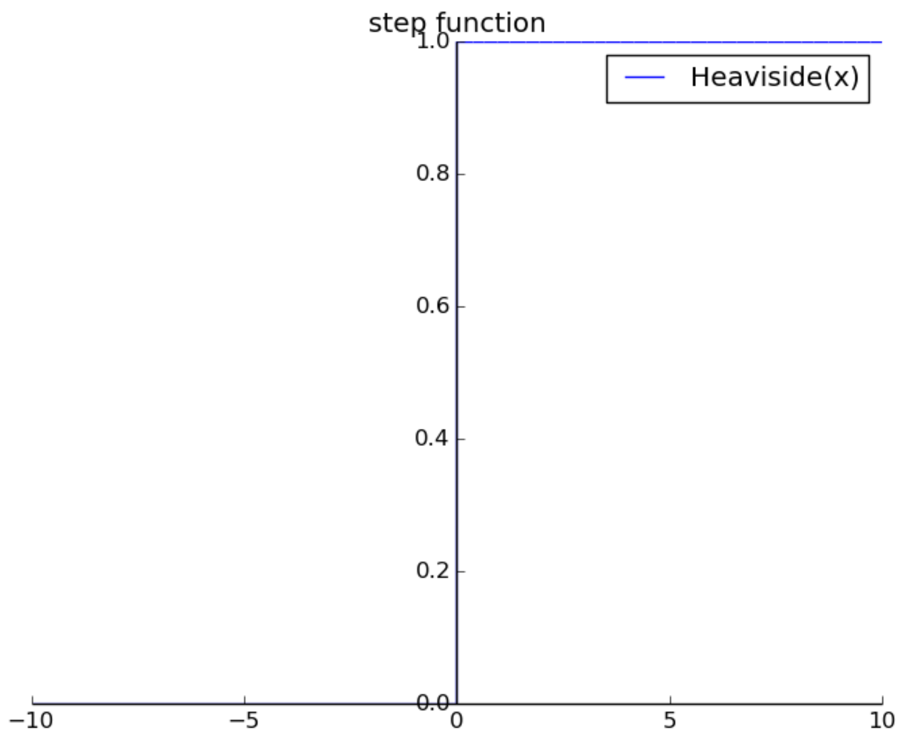


Figure 6: Step function

it much easier to figure out how changing the weights and biases will change the output.

If it's the shape of σ which really matters, and not its exact form, then why use the particular form used for σ ? In fact, there are other activation functions as well. The main thing that changes when we use a different activation function is that the particular values for the partial derivatives in Equation (5) change. It turns out that when we compute those partial derivatives, using σ will simplify the algebra.

$$\begin{aligned}\frac{d\sigma}{dz} &= \left(1 - \frac{1}{1+e^{-z}}\right)\left(\frac{1}{1+e^{-z}}\right) \\ &= (1-\sigma)\sigma\end{aligned} \tag{6}$$

1.3. The architecture of neural networks

Suppose we have the network:

As mentioned earlier, the leftmost layer in this network is called the input layer, and the neurons within the layer are called input neurons. The rightmost or output layer contains the output neurons, or, as in this case, a single output neuron. The middle layer is called a hidden layer, since the neurons in this layer are neither inputs nor outputs. The network above has just a single hidden

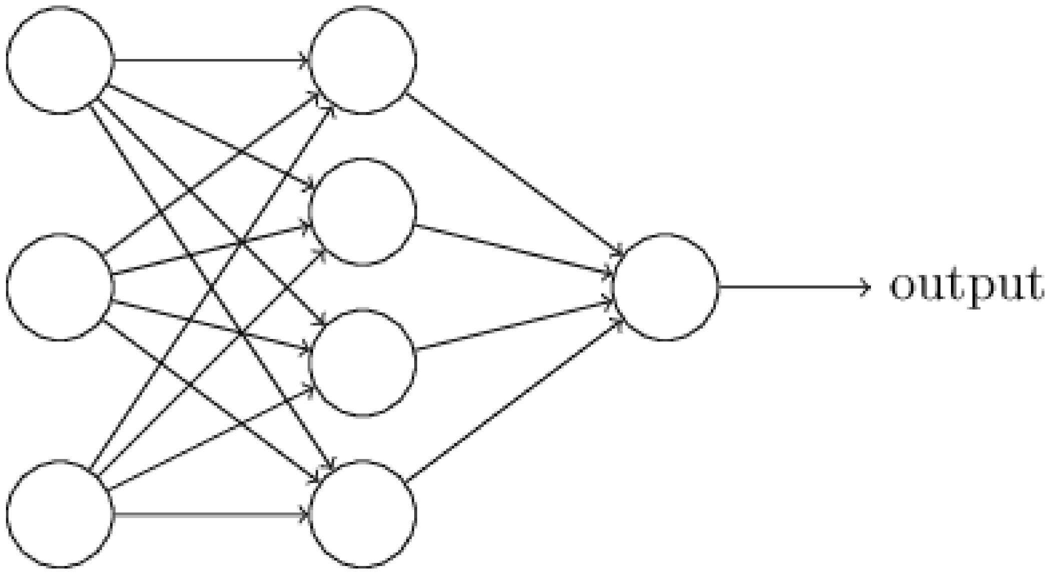


Figure 7: Simple architecture

layer, but some networks have multiple hidden layers. For example, the following four-layer network has two hidden layers:

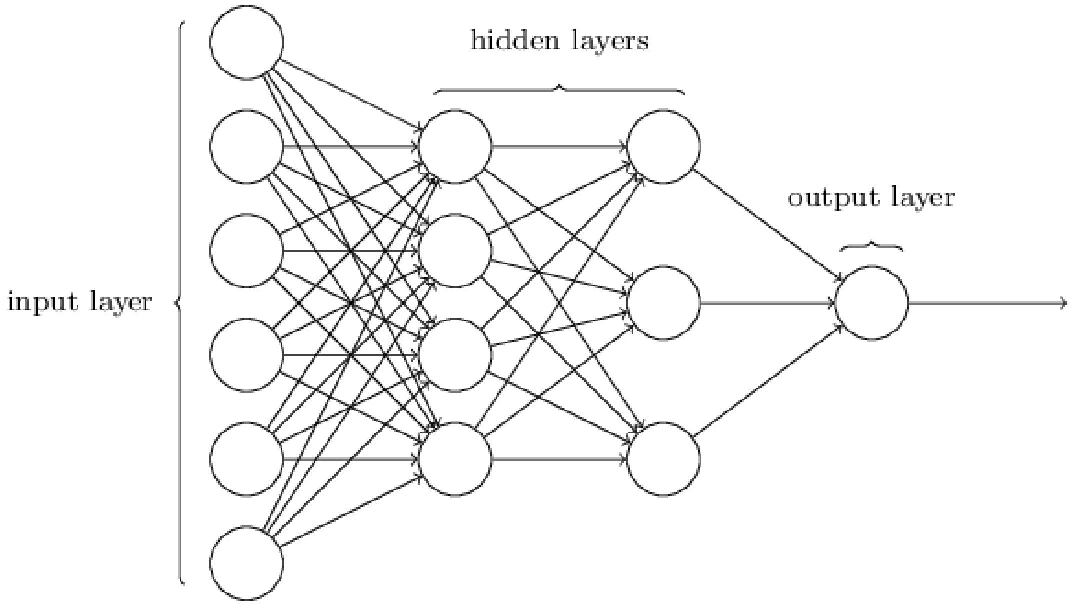


Figure 8: Layers

Somewhat confusingly, and for historical reasons, such multiple layer networks are sometimes called multilayer perceptrons or MLPs, despite being made up of sigmoid neurons, not perceptrons. It is not going to be used the MLP terminology in this article, since it is confusing.

There can be quite an art to the design of the hidden layers. Neural networks researchers have developed many design heuristics for the hidden layers, which help people get the behaviour they want out of their nets. For example, such heuristics can be used to help determine how to trade off the number of hidden layers against the time required to train the network.

Up to now, we've been discussing neural networks where the output from one layer is used as input to the next layer. Such networks are called feedforward neural networks. This means there are no loops in the network - no feedback-. Loops would be problematic in for example sigmoid neurons because of the inputs would depend on the outputs. However, there are other models of artificial neural networks in which feedback loops are possible. These models are called recurrent neural networks. The idea in these models is to have neurons which fire for some limited duration of time, before becoming quiescent. That firing can stimulate other neurons, which may fire a little while later, also for a limited duration. That causes still more neurons to fire, and so over time we get a cascade of neurons firing. Loops don't cause problems in such a model, since a neuron's output only affects its input at some later time, not instantaneously.

Recurrent neural nets have been less influential than feedforward networks, in part because the learning algorithms for recurrent nets are (at least to date) less powerful. But recurrent networks are still extremely interesting. They're much closer in spirit to how our brains work than feedforward networks. And it's possible that recurrent networks can solve important problems which can only be solved with great difficulty by feedforward networks.

1.4. A simple network to classify handwritten digits

We can split the problem of recognizing handwritten digits into two sub-problems. First, we'd like a way of breaking an image containing many digits into a sequence of separate images, each containing a single digit.

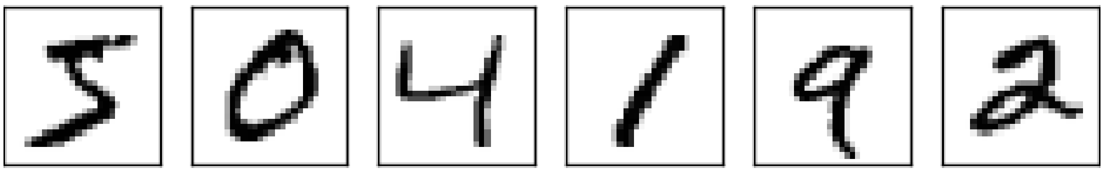


Figure 9: Seperate digits

Once the image has been segmented, the program then needs to classify each individual digit. We will focus on writing a program to classify individual digits..

To recognize individual digits we will use a three-layer neural network:

As discussed in the next section, our training data for the network will consist of many 28 by 28 pixel images of scanned handwritten digts, and so the input layer contains $784 = 28 \times 28$ neurons. The input pixels are grayscale, with a value of 0.0 representing white, a value of 1.0 representing black, and in between values representing gradually darkening shades of grey.

The second layer of the network is a hidden layer. We denote the number of neurons in this hidden layer by n, and we'll experiment with different values for n.

Why we use 10 output neurons. After all, the goal of the network is to tell us which digit $(0, 1, 2, \ldots, 9)$ corresponds to the input image. A seemingly natural way of doing that is to use just 4 output neurons, treating each neuron as taking

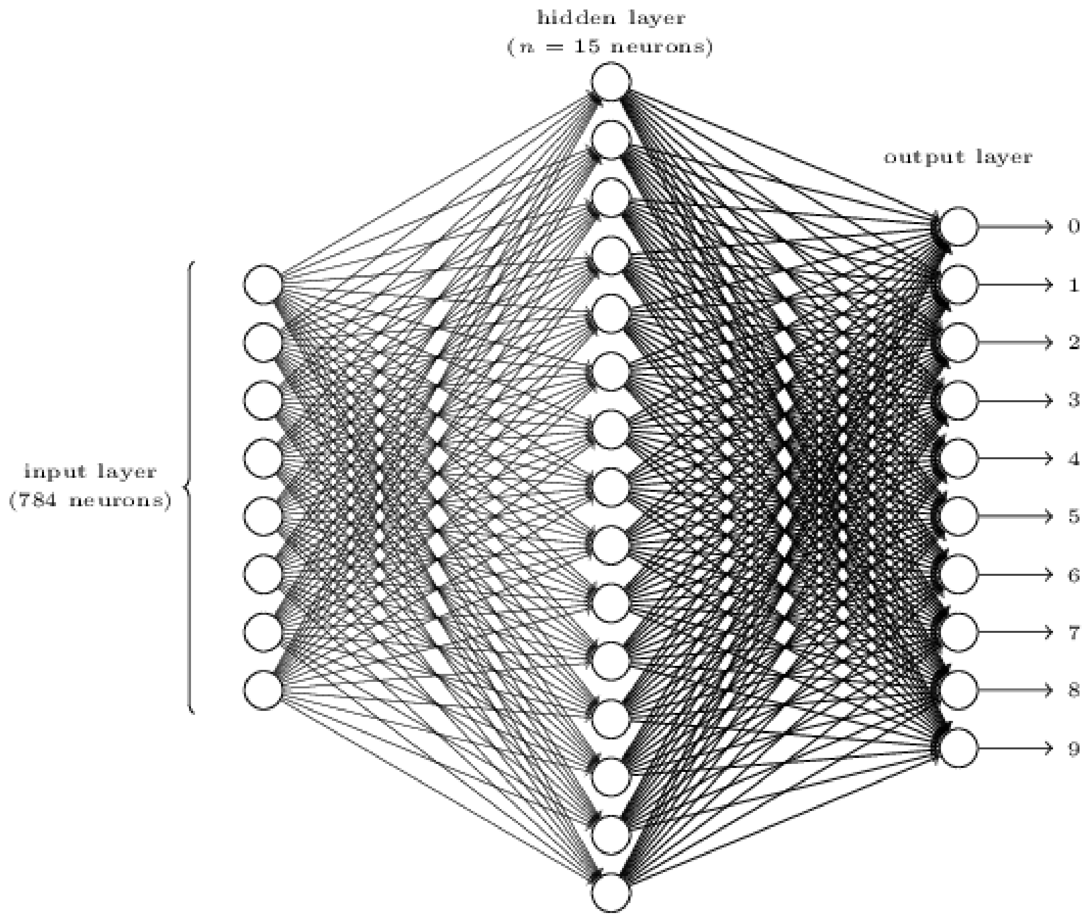


Figure 10: Three layered feedforward network

on a binary value, depending on whether the neuron's output is closer to 0 or to 1. Four neurons are enough to encode the answer, since $2^4 = 16$ is more than 10 possible values for the input digit. Why should our network use 10 neurons instead? The ultimate justification is empirical. We can try out both network designs, and it turns out that, for this particular problem, the network with 10 output neurons learns to recognize digits better than the network with 4 output neurons. But that leaves us wondering why using 10 output neurons works better?

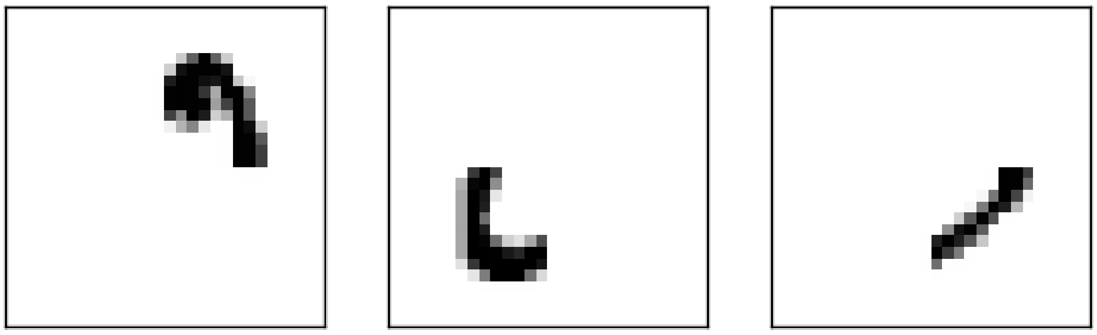


Figure 11: Some parts of number 0

First neuron in the hidden layer may detect just whether or not an image like the above is present. If we had 4 outputs, then the first output neuron would be trying to decide what the most significant bit of the digit was. And there's no easy way to relate that most significant bit to simple shapes like those shown above. However there could be always such structures with 4 neurons at the output so that net were more efficient. Now, with all that said, this is all just a heuristic.

1.5. Learning with gradient descent

Now the first thing we'll need is a data set to learn from so-called training data set. We'll use the MNIST data set which contains tens of thousands of scanned images of handwritten digits, together with their correct classifications. Images are the same as used before.

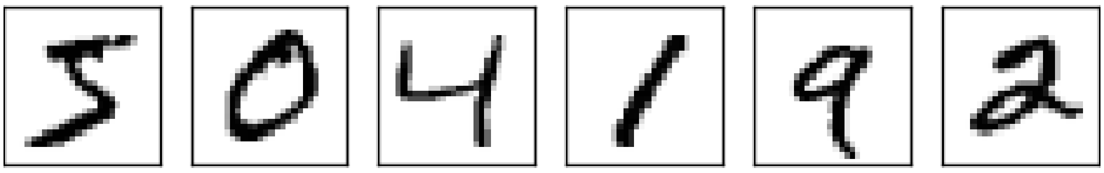


Figure 12: MNIST data set samples

The MNIST data comes in two parts. The first part contains 60,000 images to be used as training data. These images are scanned handwriting samples from 250 people, half of whom were US Census Bureau employees, and half of whom were high school students. The images are grayscale and 28 by 28 pixels in size. The second part of the MNIST data set is 10,000 images to be used as test data. Again, these are 28 by 28 grayscale images. We'll use the test data to evaluate how well our neural network has learned to recognize digits. To make this a good test of performance, the test data was taken from a different set of 250 people than the original training data (albeit still a group split between Census Bureau employees and high school students). This helps give us confidence that our system can recognize digits from people whose writing it didn't see during training.

We'll use the notation x to denote a training input. It'll be convenient to regard each training input x as a $28 \times 28 = 784$ dimensional vector. Each entry in the vector represents the gray value for a single pixel in the image. We'll denote the corresponding desired output by $y = y(x)$, where y is a 10-dimensional vector. For example, if a particular training image, x, depicts a 6, then $y(x) = (0, 0, 0, 0, 0, 0, 1, 0, 0, 0)^T$ is the desired output from the network. Note that T here is the transpose operation, turning a row vector into an ordinary (column) vector.

What we'd like is an algorithm which lets us find weights and biases so that the output from the network approximates $y(x)$ for all training inputs x. To quantify how well we're achieving this goal we define a cost function. Sometimes referred to as a loss or objective function.

$$C(w,\ b) \equiv \frac{1}{2n} \sum_x ||y(x) - a||^2 \tag{7}$$

Here, w denotes the collection of all weights in the network, b all the biases, n is the total number of training inputs, a is the vector of outputs from the network when x is input, and the sum is over all training inputs, x. Of course, the output a depends on x, w and b. The notation $||v||$ just denotes the usual length function for a vector v. We'll call C the quadratic cost function; it's also sometimes known as the mean squared error orjust MSE. $C(w,\ b)$ is non-negative, since every term in the sum is non-negative. Furthermore, the cost $C(w,\ b)$ precisely when $y(x)$ is approximately equal to the output, a, for all training inputs, x. So our training algorithm has done a good job if it can find weights and biases so that $C(w,\ b) \approx 0$. By contrast, it's not doing so well when $C(w,\ b)$ is large - that would mean that $y(x)$ is not close to the output a for a large number of inputs. So the aim of our training algorithm will be to minimize the cost $C(w,\ b)$ as a function of the weights and biases.

Okay, let's suppose we're trying to minimize some function, $C(v)$. This could be any real-valued function of many variables, $v = v_1, v_2, \ldots$

What we'd like is to find where C achieves its global minimum. One way of attacking the problem is to use calculus to try to find the minimum analytically. With some luck that might work when C is a function of just one or a few variables. But it'll turn into a nightmare when we have many more variables. And for neural networks we'll often want far more variables - the biggest neural networks have cost functions which depend on billions of weights and biases in an extremely complicated way. Using calculus to minimize that just won't work! We start by thinking of our function as a kind of a valley. And we imagine a ball rolling down the slope of the valley. Our everyday experience tells us that the ball will eventually roll to the bottom of the valley.

Let's think about what happens when we move the ball a small amount Δv_1 in the v_1 direction, and a small amount Δv_2 in the v_2 direction. Calculus tells us that C changes as follows:

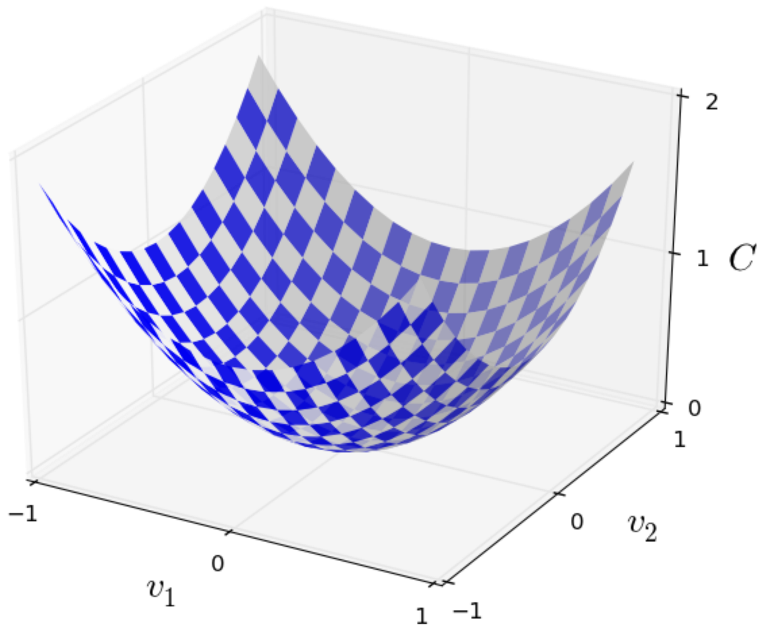


Figure 13: Sample cost function with double variables

$$\Delta C \approx \frac{\partial C}{\partial v_1}\Delta v_1 + \frac{\partial C}{\partial v_2}\Delta v_2 \tag{8}$$

We're going to find a way of choosing Δv_1 and Δv_2 so as to make ΔC negative; i.e., we'll choose them so the ball is rolling down into the valley. To figure out how to make such a choice it helps to define Δv to be the vector of changes in v, $\Delta v \equiv (\Delta v_1,\ \Delta v_2)^T$. We denote the gradient vector by ∇C, i.e.:

$$\nabla C \equiv \left(\frac{\partial C}{\partial v_1}, \frac{\partial C}{\partial v_2}\right)^T \tag{9}$$

More generally, if C is function of m variables,

$$\nabla C \equiv \left(\frac{\partial C}{\partial v_1}, \frac{\partial C}{\partial v_2}, \ ..., \ \frac{\partial C}{\partial v_m}\right)^T \tag{10}$$

With these definitions, the expression (8) for ΔC can be rewritten as

$$\Delta C \approx \nabla C \Delta v \tag{11}$$

In particular, suppose we choose,

$$\Delta v = \eta \nabla C \tag{12}$$

where η is a small, positive parameter (known as the learning rate). Then Equation (11) becomes

$$\Delta C \approx \eta \nabla C \cdot \nabla C = \eta ||\nabla C||^2 \tag{13}$$

This guarantees that $\Delta C \leq 0$, i.e., C will always decrease. This is exactly the property we wanted! And so we'll take Equation (12) to define the "law of motion" for the ball in our gradient descent algorithm. That is, we'll use Equation (12) to compute a value for Δv, then move the ball's position v by that amount:

$$v \rightarrow v' = v \eta \nabla C \tag{14}$$

Then we'll use this update rule again, to make another move. If we keep doing this, over and over, we'll keep decreasing C until - we hope - we reach a global minimum.

Summing up, the way the gradient descent algorithm works is to repeatedly compute the gradient ∇C, and then to move in the opposite direction, "falling down" the slope of the valley.

To make gradient descent work correctly, we need to choose the learning rate η to be small enough that Equation (12) is a good approximation. If we don't, we might end up with $\Delta C > 0$, which obviously would not be good! At the same time, we don't want η to be too small, since that will make the changes Δv tiny, and thus the gradient descent algorithm will work very slowly.

Unfortunately, this rule does not always work - several things can go wrong and prevent gradient descent from finding the global minimum of C, a point we'll return to explore in later chapters. But, in practice gradient descent often works extremely well, and in neural networks we'll find that it's a powerful way of minimizing the cost function, and so helping the net learn.

How can we apply gradient descent to learn in a neural network? The idea is to use gradient descent to find the weights w_k and biases b_l which minimize the cost in Equation (7). To see how this works, let's restate the gradient descent update rule, with the weights and biases replacing the variables v_j.

$$\begin{aligned} w_k \rightarrow w_k' &= w_k \eta \frac{\partial C}{\partial w_k} \\ b_l \rightarrow b_l' &= b_l \eta \frac{\partial C}{\partial b_l} \end{aligned} \tag{15}$$

By repeatedly applying this update rule we can "roll down the hill", and hopefully find a minimum of the cost function. In other words, this is a rule which can be used to learn in a neural network.

Notice that this cost function has the form $C = \frac{1}{n} \sum_x C_x$, that is, it's an average over costs $C_x \equiv \frac{||y(x)-a||^2}{2}$ for individual training examples. In practice, to compute the gradient ∇C we need to compute the gradients ∇C_x separately for each training input, x, and then average them, $\nabla C = \frac{1}{n} \sum_x \nabla C_x$. Unfortunately, when the number of training inputs is very large this can take a long time, and learning thus occurs slowly.

An idea called stochastic gradient descent can be used to speed up learning. The idea is to estimate the gradient ∇C by computing ∇C_x for a small sample of randomly chosen training inputs. By averaging over this small sample it turns out that we can quickly get a good estimate of the true gradient ∇C, and this helps speed up gradient descent, and thus learning.

To make these ideas more precise, stochastic gradient descent works by randomly picking out a small number m of randomly chosen training inputs. We'll label those random training inputs $X_1, X_2, \ldots, X_m$ and refer to them as a mini-batch.

$$\nabla C \approx \frac{1}{m} \sum_{j=1} \nabla C_{X_j} \tag{16}$$

Equation (16) depicts that overall gradient can be estimated just by randomly chosen mini-batch. And updating weights and biases is like below

$$\begin{aligned} w_k \rightarrow w_k' &= w_k \frac{\eta}{m} \sum_j \frac{\partial C_{X_j}}{\partial w_k} \\ b_l \rightarrow b_l' &= b_l \frac{\eta}{m} \sum_j \frac{\partial C_{X_j}}{\partial b_l} \end{aligned} \tag{17}$$

where the sums are over all the training examples X_j in the current mini-batch. Then we pick out another randomly chosen mini-batch and train with those. And so on, until we've exhausted the training inputs, which is said to complete an epoch of training. At that point we start over with a new training epoch.

It's much easier to sample a small mini-batch than it is to apply gradient descent to the full batch. For example, if we have a training set of size $n = 60,000$, as in MNIST, and choose a mini-batch size of (say) $m = 10$, this means we'll get a factor of 6,000 speedup in estimating the gradient! Of course, the estimate won't be perfect - there will be statistical fluctuations - but it doesn't need to be perfect: all we really care about is moving in a general direction that will help decrease C, and that means we don't need an exact computation of the gradient. In practice, stochastic gradient descent is a commonly used and powerful technique for learning in neural networks.

1.6. Implementing our network to classify digits

Get the codes from https://github.com/mnielsen/neural-networks-and-deep-learning

First MNIST must be loaded.

```
>>>import mnist_loader
>>>training_data, validation_data, test_data = \
mnist_loader.load_data_wrapper()
```

Then,

```
>>>import network
>>>net = network.Network([784, 30, 10])
```

Finally, we'll use stochastic gradient descent to learn from the MNIST training data over 30 epochs, with a mini-batch size of 10, and a learning rate of $\eta = 3.0$,

```
>>>net.SGD(training_data,30,10,3.0,test_data=test_data)
```

The results are,

```
Epoch 0: 9129 / 10000
Epoch 1: 9295 / 10000
Epoch 2: 9348 / 10000
...
Epoch 27: 9528 / 10000
Epoch 28: 9542 / 10000
Epoch 29: 9534 / 10000
```

That is, the trained network gives us a classification rate of about 95 percent - 95.42 percent at its peak ("Epoch 28")! That's quite encouraging as a first attempt. However, that if you run the code then your results are not necessarily going to be quite the same as mine, since we'll be initializing our network using (different) random weights and biases.

Choosing the learning rate η too low i.e. $\eta = 0.001$, causes slowly convergence and you may not get good results in reasonable epoch numbers like 100 epochs. On the other hand choosing η too high i.e. $\eta = 100$ causes to divergence continuously and you get very low accurate results.

Learning rate, epoch number, mini batch-size etc. are hyper parameters. You can adjust these parameters and may get better and faster results.

2. How the backpropagation algorithm works

The backpropagation algorithm was originally introduced in the 1970s, but its importance wasn't fully appreciated until a famous 1986 paper by David Rumelhart, Geoffrey Hinton, and Ronald Williams. That paper describes several neural networks where backpropagation works far faster than earlier approaches to learning, making it possible to use neural nets to solve problems which had previously been insoluble. Today, the backpropagation algorithm is the workhorse of learning in neural networks.

2.1. A fast matrix-based approach to computing the output from a neural network

We'll use w^l_{jk} to denote the weight for the connection from the k^{th} neuron in the $(l1)^{th}$ layer to the j^{th} neuron in the l^{th} layer. So, for example, the diagram below shows the weight on a connection from the fourth neuron in the second layer to the second neuron in the third layer of a network:

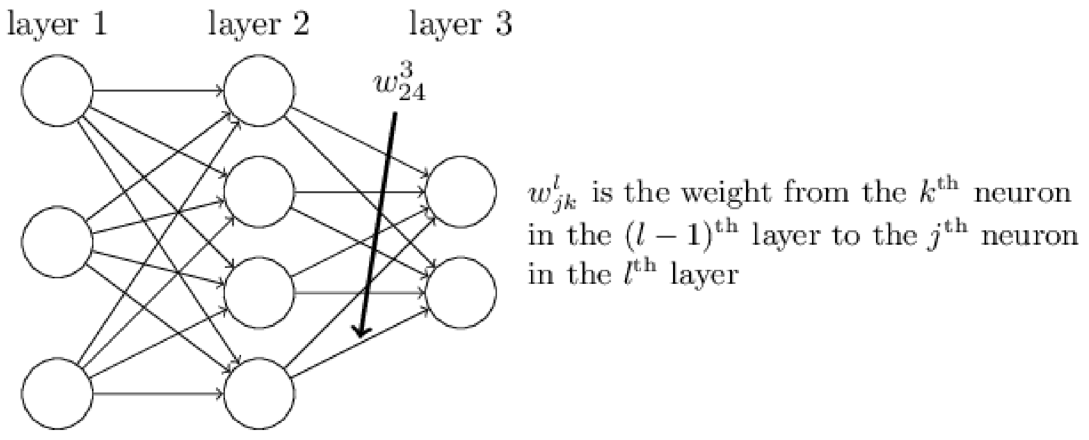

layer 1
layer 2
layer 3
w^3_{24}
w^l_{jk} is the weight from the k^{th} neuron in the $(l-1)^{\text{th}}$ layer to the j^{th} neuron in the l^{th} layer

Figure 14: Weight notation

We use a similar notation for the network's biases and activations. Explicitly, we use b^l_j for the bias of the j^{th} neuron in the l^{th} layer. And we use a^l_j for the activation of the j^{th} neuron in the l^{th} layer. The following diagram shows examples of these notations in use:

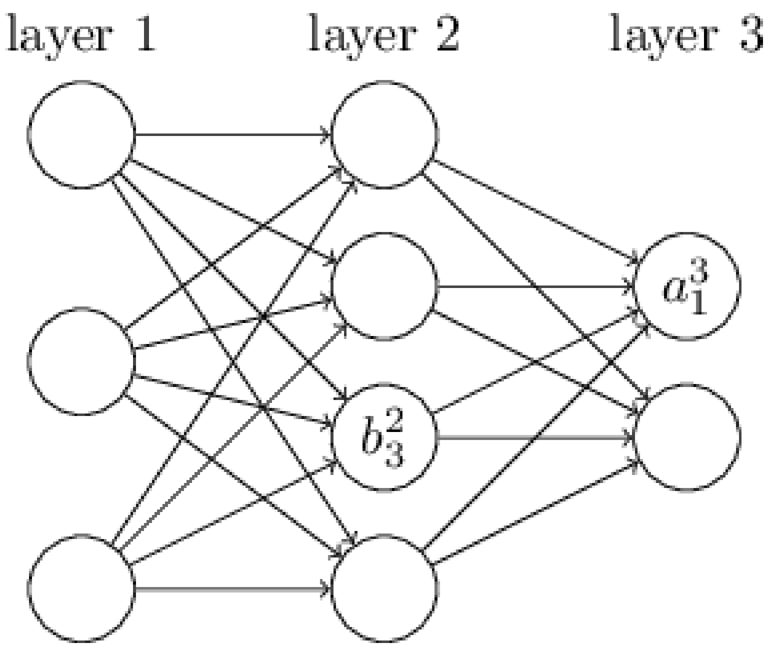


Figure 15: Bias and activation notation

The activation a^l_j of the j^{th} neuron in the l^{th} layer is related to the activations in the $(l-1)^{th}$ layer by the equation

$$a^l_j = \sigma(\sum_k w^l_{jk} a^{l-1}_k + b^l_j) \tag{18}$$

where the sum is over all neurons k in the $(l-1)^{th}$ layer. Equation (18) can be rewritten in the beautiful and compact vectorized form

$$a^l = \sigma(w^l \cdot a^{l-1} + b^l) \tag{19}$$

This expression gives us a much more global way of thinking about how the activations in one layer relate to activations in the previous layer: we just apply the weight matrix to the activations, then add the bias vector, and finally apply the σ function. The expression is also useful in practice, because most matrix libraries provide fast ways of implementing matrix multiplication, vector addition, and vectorization.

2.2. The Hadamard product, $s \odot t$

Suppose s and t are two vectors of the same dimension. Then we use $s \odot t$ to denote the elementwise product of the two vectors. Thus the components of $s \odot t$ are just $s \odot t_j = s_j t_j$. As an example,

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \odot \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \times 3 \\ 2 \times 4 \end{bmatrix} = \begin{bmatrix} 3 \\ 8 \end{bmatrix} \tag{20}$$

This kind of elementwise multiplication is sometimes called the Hadamard product or Schur product. Good matrix libraries usually provide fast implementations of the Hadamard product, and that comes in handy when implementing backpropagation.

2.3. The four fundamental equations behind backpropagation

We first introduce an intermediate quantity, δ^l_j, which we call the error in the j^{th} neuron in the l^{th} layer. Backpropagation will give us a procedure to compute the error δ^l_j, and then will relate it to $\partial C / \partial w^l_{jk}$ and $\partial C / \partial b^l_j$.

We define the error δ^l_j of neuron j in layer l by

$$\delta^l_j \equiv \frac{\partial C}{\partial z^l_j} \tag{21}$$

Backpropagation is based around four fundamental equations. Together, those equations give us a way of computing both the error δ^l and the gradient of the cost function.

An equation for the error in the output layer, δ^L: The components of δ^L are given by

$$\delta_j^L = \frac{\partial C}{\partial a_j^L}\sigma'(z_j^L) \tag{22}$$

This is a very natural expression. The first term on the right, $\partial C/\partial a_j^L$, just measures how fast the cost is changing as a function of the j^{th} output activation. If, for example, C doesn't depend much on a particular output neuron, j, then δ_j^L will be small, which is what we'd expect. The second term on the right, $\sigma' z_j^L)$, measures how fast the activation function σ is changing at z_j^L. If we're using the quadratic cost function then $C = \frac{1}{2}\sum_j (y_j - a_j)^2$, and so $\partial C/\partial a_j^L = (a_j - y_j)$, which obviously is easily computable.

It's easy to rewrite the Equation (22) in a matrix-based form, as

$$\delta^L = (a^L - y) \odot \sigma'(z^L) \tag{23}$$

An equation for the error δ^l in terms of the error in the next layer, $\delta_l + 1$: In particular

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l) \tag{24}$$

We can think intuitively of this as moving the error backward through the network, giving us some sort of measure of the error at the output of the l^{th} layer.

By combining (23) with (24) we can compute the error δ^l for any layer in the network. We start by using (23) to compute δ^L, then apply Equation (24) to compute δ^{L-1}, then δ^{L-2}, and so on, all the way back through the network.

An equation for the rate of change of the cost with respect to any bias in the network: In particular:

$$\frac{\partial C}{\partial b_j^l} = \delta_j^l \tag{25}$$

or in shorthand as

$$\frac{\partial C}{\partial b} = \delta \tag{26}$$

where it is understood that δ is being evaluated at the same neuron as the bias b.

An equation for the rate of change of the cost with respect to any weight in the network: In particular:

$$\frac{\partial C}{\partial w_{jk}^l} = a_k^{l-1}\delta_j^l \tag{27}$$

This tells us how to compute the partial derivatives $\partial C/\partial w_{jk}^l$ in terms of the quantities δ^l and a^{l-1}, which we already know how to compute. The equation can be rewritten in a less index-heavy notation as

$$\frac{\partial C}{\partial w} = a_{in}\delta_{out} \tag{28}$$

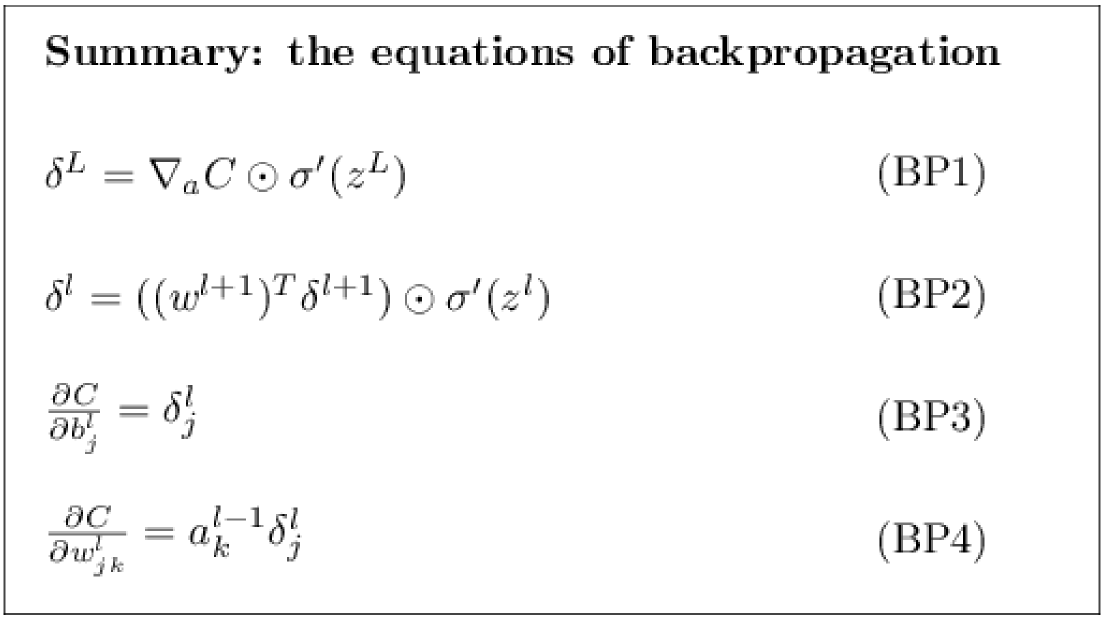
where it's understood that a_{in} is the activation of the neuron input to the weight w, and δ_{out} is the error of the neuron output from the weight w.

A nice consequence of Equation (28) is that when the activation a_{in} is small, $a_{in} \approx 0$, the gradient term $\partial C/\partial w$ will also tend to be small. In this case, we'll say the weight learns slowly, meaning that it's not changing much during gradient descent. In other words, one consequence of (28) is that weights output from low-activation neurons learn slowly.

Recall from the graph of the sigmoid function in the last chapter that the σ function becomes very flat when $\sigma(z_j^L)$ is approximately 0 or 1. When this occurs we will have $\sigma'(z_j^L) \approx 0$. And so the lesson is that a weight in the final layer will learn slowly if the output neuron is either low activation (≈ 0) or high activation (≈ 1).

Summing up, we've learnt that a weight will learn slowly if either the input neuron is low-activation, or if the output neuron has saturated, i.e., is either high- or low-activation.

The four fundamental equations turn out to hold for any activation function, not just the standard sigmoid function (that's because, the proofs don't use any special properties of). And so we can use these equations to design activation functions which have particular desired learning properties. As an example to give you the idea, suppose we were to choose a (non-sigmoid) activation function σ so that σ' is always positive, and never gets close to zero. That would prevent the slow-down of learning that occurs when ordinary sigmoid neurons saturate.



Summary: the equations of backpropagation

$$\delta^L = \nabla_a C \odot \sigma'(z^L) \tag{BP1}$$

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l) \tag{BP2}$$

$$\frac{\partial C}{\partial b_j^l} = \delta_j^l \tag{BP3}$$

$$\frac{\partial C}{\partial w_{jk}^l} = a_k^{l-1}\delta_j^l \tag{BP4}$$

Figure 16: Four fundamental equations of backpropapagation

The proof of four fundamental equations of backpropagation is just coming from systematically applying the chain rule to the cost function so that we may be able to get gradients of it.

2.4. The backpropagation algorithm

The backpropagation equations provide us with a way of computing the gradient of the cost function. Let's explicitly write this out in the form of an algorithm:

1. Input x: Set the corresponding activation a^1 for the input layer.
2. Feedforward: For each $l = 2, 3, \dots, L$ compute $z^l = w^l a^{l-1} + b^l$ and $a^l = \sigma(z^l)$.
3. Output error δ^L: Compute the vector $\delta^L = \nabla_a C \odot \sigma'(z^L)$.
4. Backpropagate the error: For each $l = L-1, L-2, \dots, 2$ compute $\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$.
5. Output: The gradient of the cost function is given by $\frac{\partial C}{\partial w^l_{jk}} = a^{l-1} \sum_k \delta^l_j$ and $\frac{\partial C}{\partial b^l_j} = \delta^l_j$.

Examining the algorithm you can see why it's called backpropagation. We compute the error vectors δ^l backward, starting from the final layer. The backward movement is a consequence of the fact that the cost is a function of outputs from the network. To understand how the cost varies with earlier weights and biases we need to repeatedly apply the chain rule, working backward through the layers to obtain usable expressions.

In practice, it's common to combine backpropagation with a learning algorithm such as stochastic gradient descent, in which we compute the gradient for many training examples. In particular, given a mini-batch of m training examples, the following algorithm applies a gradient descent learning step based on that mini-batch:

1. Input a set of training examples
2. For each training example x: Set the corresponding input activation $a^{x,1}$, and perform the following steps:
3. Feedforward: For each $l = 2, 3, \dots, L$ compute $z^{x,l} = w^l a^{x,l-1} + b^l$ and $a^{x,l} = \sigma(z^{x,l})$.
4. Output error $\delta^{x,L}$: Compute the vector $\delta^{x,L} = \nabla_a C_x \odot \sigma'(z^{x,L})$.
5. Backpropagate the error: For each $l = L-1, L-2, \dots, 2$ compute $\delta^{x,l} = ((w^{l+1})^T \delta^{x,l+1}) \odot \sigma'(z^{x,l})$.
6. Gradient descent: For each $l = L, L-1, \dots, 2$ update the weights according to the rule $w^l \rightarrow w^l - \frac{\eta}{m} \sum_x \delta^{x,l} (a^{x,l-1})^T$, and the biases according to the rule $b^l \rightarrow b^l - \frac{\eta}{m} \sum_x \delta^{x,l}$.

Of course, to implement stochastic gradient descent in practice you also need an outer loop generating mini-batches of training examples, and an outer loop stepping through multiple epochs of training.

3. Improving the way neural networks learn

In this chapter it's explained a suite of techniques which can be used to improve the implementation of backpropagation, and so improve the way our networks learn.

The techniques we'll develop in this chapter include: a better choice of cost function, known as the cross-entropy cost function; four "regularization" methods (L1 and L2 regularization, dropout, and artificial expansion of the training data), which make our networks better at generalizing beyond the training data; a better method for initializing the weights in the network; and a set of heuristics to help choose good hyper-parameters for the network.

3.1. The cross-entropy cost function

Ideally, we hope and expect that our neural networks will learn fast from their errors. Is this what happens in practice? To answer this question, let's look at a toy example. The example involves a neuron with just one input:

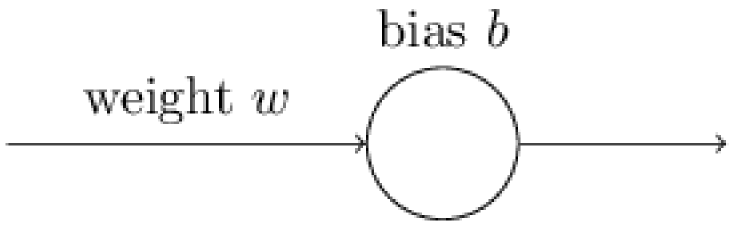


Figure 17: Simple neuron

We'll train this neuron taking the input 1 to the output 0. Of course, this is such a trivial task that we could easily figure out an appropriate weight and bias by hand, without using a learning algorithm. However, it turns out to be illuminating to use gradient descent to attempt to learn a weight and bias. So let's take a look at how the neuron learns.

To make things definite, we'll pick the initial weight to be 0.6 and the initial bias to be 0.9 generically. The initial output from the neuron is 0.82, so quite a bit of learning will be needed before our neuron gets near the desired output, 0.0. The learning rate is $\eta = 0.15$. The cost is the quadratic cost function, C. Code and the result shown below.

```
import matplotlib.pylab as plt
import numpy as np

class Sigmoid(object):

    def activate(self, z):
        return 1. / (1. + np.exp(-z))

    def diff(self, z):
        return self.activate(z) * (1. - self.activate(z))

class QuadraticCost(object):

    def cost(self, y, out):
        return 0.5 * ((y - out)  2.)

    def diff(self, y, out):
        return (out - y)

class CrossEntropyCost(object):

    def cost(self, y, out):
        return -(y  np.log(out) + (1. - y) * np.log(1. - out))

    def diff(self, y, out):
        return (y - out) / (out * (out - 1.))

def singleNeuronModel(weight, bias, x=1.0, y=0.0, \
                      costFunction=QuadraticCost(),
                      eta=0.15, \
                      activationFunction=Sigmoid(), \
                      epoch=300):
'''
Models a single neuron for given weight and bias.
Input x = 1.0 and expected output y = 0.0.
Learning rate eta = 0.15.
Epoch (total training number) is 300.
'''
allCosts = []
for i in range(epoch):
    z = x  weight + bias
    out = activationFunction.activate(z)
    weight -= eta * costFunction.diff(y, out) * \
              activationFunction.diff(z) * out
    bias -= eta * costFunction.diff(y, out) * \
            activationFunction.diff(z)
    allCosts.append(costFunction.cost(y, out))

# Last out value with updated weights and biases.
z = x * weight + bias
out = activationFunction.activate(z)
allCosts.append(costFunction.cost(y, out))

# Print last weight, bias and output and drawing.
print "weight: {}, bias: {}, output: {}".format \
      (weight, bias, allCosts[-1])
plt.plot(range(epoch + 1), allCosts)
plt.xlabel('epochs')
plt.ylabel('cost')
plt.show()
```

```
singleNeuronModel(weight=0.6, bias=0.9)
```

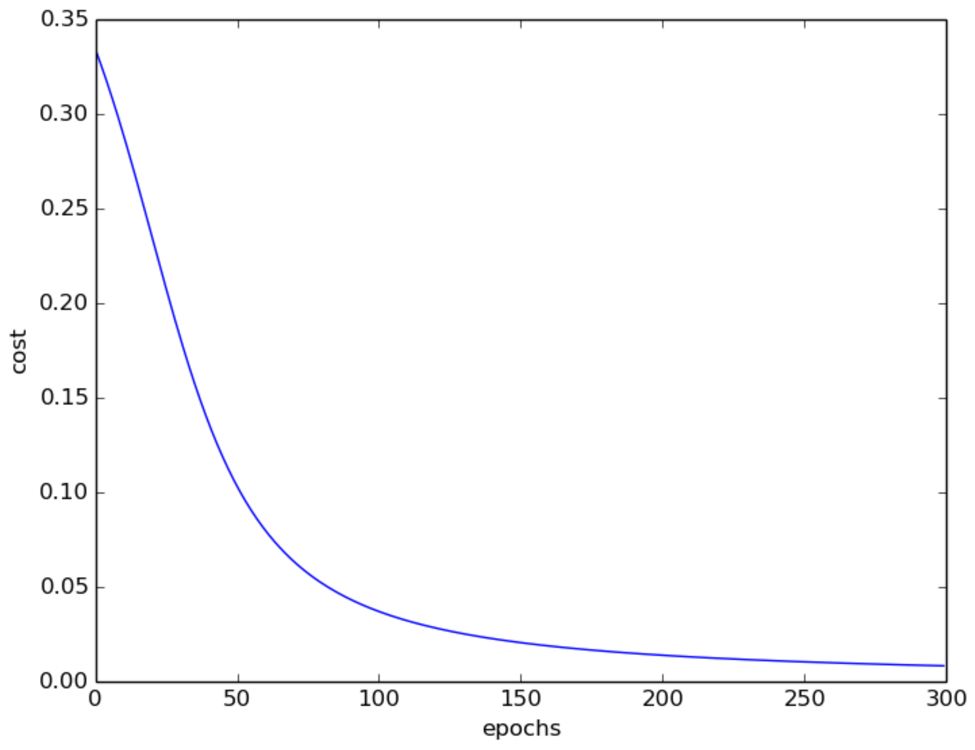


Figure 18: Single neuron with weight=0.6, bias=0.9

As you can see, the neuron rapidly learns a weight and bias that drives down the cost, and gives an output 0.008. Suppose, however, that we instead choose both the starting weight and the starting bias to be 2.0. In this case the initial output is 0.98, which is very badly wrong. Let's look at how the neuron learns to output 0 in this case.

```
singleNeuronModel(weight=2.0, bias=2.0)
```

Although this example uses the same learning rate ($\eta = 0.15$), we can see that learning starts out much more slowly. Indeed, for the first 150 or so learning epochs, the weights and biases don't change much at all.

This behaviour is strange when contrasted to human learning. As I said at the beginning of this section, we often learn fastest when we're badly wrong about something. But we've just seen that our artificial neuron has a lot of difficulty learning when it's badly wrong - far more difficulty than when it's just a little

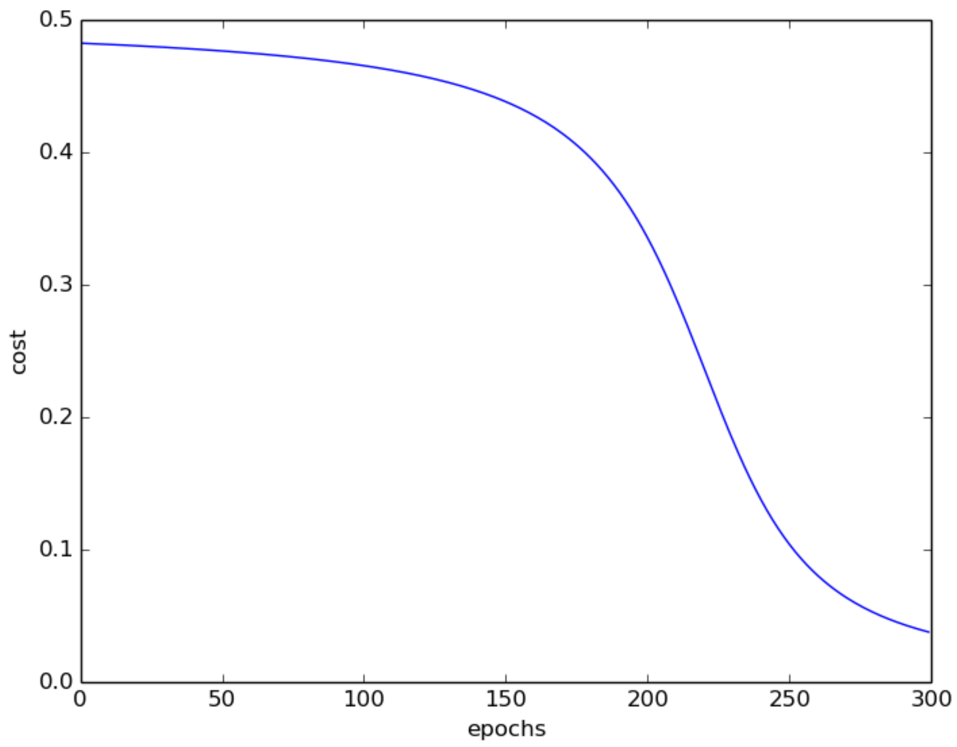


Figure 19: Single neuron with weight=2.0, bias=2.0

wrong. What's more, it turns out that this behaviour occurs not just in this toy model, but in more general networks. Why is learning so slow? And can we find a way of avoiding this slowdown?

To understand the origin of the problem, let's compute the partial derivatives. Recall that we're using the quadratic cost function,

$$C = \frac{(y-a)^2}{2} \tag{29}$$

where a is the neuron's output when the training input $x = 1$ is used, and $y = 0$ is the corresponding desired output. Recall that $a = \sigma(z)$, where $z = w \cdot x + b$. Using the chain rule to differentiate with respect to the weight and bias we get

$$\begin{aligned}\frac{\partial C}{\partial w} &= \frac{\partial C}{\partial a}\frac{\partial a}{\partial \sigma}\frac{\partial \sigma}{\partial w} = (a-y)\sigma'(z)x = a\sigma'(z)\\ \frac{\partial C}{\partial b} &= \frac{\partial C}{\partial a}\frac{\partial a}{\partial \sigma}\frac{\partial \sigma}{\partial b} = (a-y)\sigma'(z) = a\sigma'(z)\end{aligned} \tag{30}$$

where substituted $x = 1$ and $y = 0$. To understand the behaviour of these expressions, let's look more closely at the $\sigma'(z)$ term on the right-hand side. Recall the shape of the σ function:

We can see from this graph that when the neuron's output is close to 1, the curve gets very flat, and so $\sigma'(z)$ gets very small. Therefore $\partial C/\partial w$ and $\partial C/\partial b$ get very small. This is the origin of the learning slowdown.

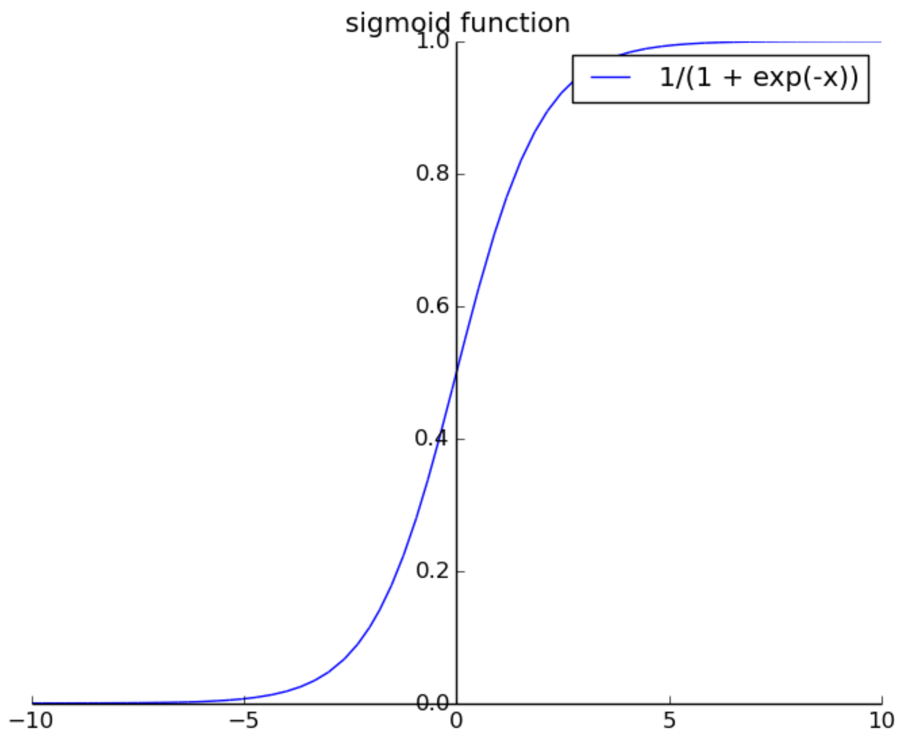


Figure 20: Sigmoid function

3.2. Introducing the cross-entropy cost function

How can we address the learning slowdown? It turns out that we can solve the problem by replacing the quadratic cost with a different cost function, known as the cross-entropy. To understand the cross-entropy, let's move a little away from our super-simple toy model. We'll suppose instead that we're trying to train a neuron with several input variables, $x_1, x_2, \ldots$ corresponding weights $w_1, w_2, \ldots$ and a bias, b:

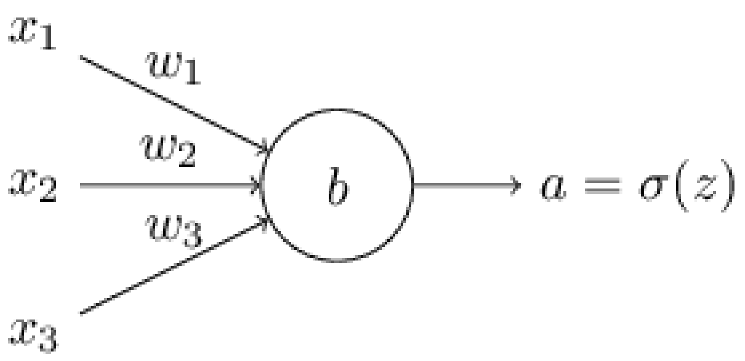


Figure 21: A neuron with multiple inputs

The output from the neuron is, of course, $a = \sigma(z)$, where $z = \sum_j w_j x_j + b$ is the weighted sum of the inputs. We define the cross-entropy cost function for this neuron by

$$C = -\frac{1}{n}\sum_x [y \ln a + (1-y)\ln(1-a)] \tag{31}$$

where n is the total number of items of training data, the sum is over all training inputs, x, and y is the corresponding desired output. The quantity $-[y \ln a + (1-y)\ln(1-a)]$ is sometimes known as the binary entropy.

Two properties in particular make it reasonable to interpret the cross-entropy as a cost function. First, it's non-negative, that is, $C > 0$. y takes only 0 or 1 and a takes values between 0 and 1. Then $\ln(1-a) < 0$ and $\ln(a) < 0$. The minus sign out of front provides $C > 0$.

Second, if the neuron's actual output is close to the desired output, i.e., $y = y(x)$ for all training inputs x , then the cross-entropy will be close to zero.

```
>>> import sympy as sp
>>> a, y = sp.symbols("a y")
>>> expr = - (y  sp.ln(a) + (1 - y)  sp.ln(1 - a))
>>> expr.subs({y:0, a:0.00001})
    1.00000500002878e-5
>>> expr.subs({y:1, a:0.99999})
    1.00000500005137e-5
```

To see this, let's compute the partial derivative of the cross-entropy cost with respect to the weights. We substitute $a = \sigma(z)$ into (31), and apply the chain rule twice, obtaining:

$$\begin{aligned}\frac{\partial C}{\partial w_j} &= -\frac{1}{n}\sum_x \left(\frac{y}{\sigma(z)} - \frac{(1-y)}{1-\sigma(z)}\right)\frac{\partial \sigma}{\partial w_j} \\ &= -\frac{1}{n}\sum_x \left(\frac{y}{\sigma(z)} - \frac{(1-y)}{1-\sigma(z)}\right)\sigma'(z)x_j \\ &= \frac{1}{n}\sum_x \frac{\sigma'(z)x_j}{\sigma(z)[1-\sigma(z)]}(\sigma(z)-y)\end{aligned} \tag{32}$$

We know that $\sigma'(z) = \sigma(z)[1-\sigma(z)]$. Therefore (32) becomes,

$$\frac{\partial C}{\partial w_j} = \frac{1}{n}\sum_x x_j[\sigma(z)-y] \tag{33}$$

This is a beautiful expression. It tells us that the larger the error, the faster the neuron will learn. In a similar way, it can be easily verified that

$$\frac{\partial C}{\partial b} = \frac{1}{n}\sum_x [\sigma(z)-y] \tag{34}$$

Let's return to the toy example we played with earlier, and explore what happens when we use the cross-entropy instead of the quadratic cost. To re-orient ourselves, we'll begin with the case where the quadratic cost did just fine, with starting weight 0.6 and starting bias 0.9.

```
singleNeuronModel(weight=0.6, bias=0.9, \
                  costFunction=CrossEntropyCost())
```

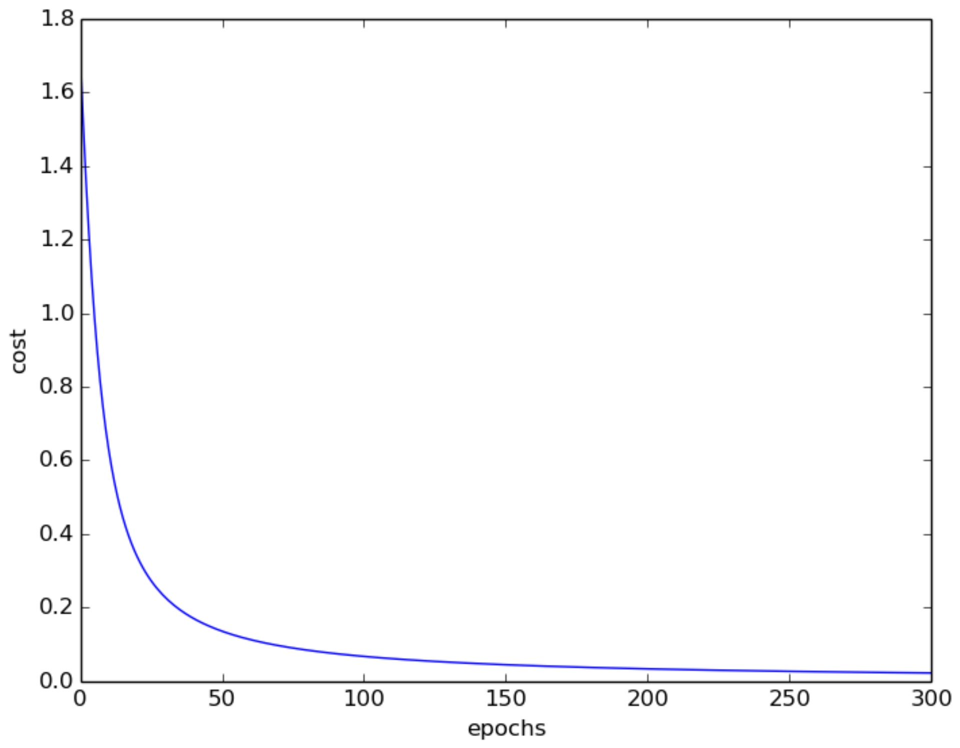


Figure 22: Single neuron with cross entropy cost with weight=0.6, bias=0.9

Now with starting weight 2.0 and starting bias 2.0.

```
singleNeuronModel(weight=2.0, bias=2.0, \
                  costFunction=CrossEntropyCost())
```

Success! This time the neuron learned quickly, just as we hoped.

We've been studying the cross-entropy for a single neuron. However, it's easy to generalize the cross-entropy to many-neuron multi-layer networks. In particular, suppose $y = y_1, y_2, \ldots$ are the desired values at the output neurons, i.e., the neurons in the final layer, while $a_1^L, a_2^L, \ldots$ are the actual output values. Then we define the cross-entropy by

$$C = -\frac{1}{n} \sum_x \sum_j \left[y_j \ln a_j^L + (1 - y_j) \ln(1 - a_j^L) \right] \tag{35}$$

When should we use the cross-entropy instead of the quadratic cost? In fact, the cross-entropy is nearly always the better choice, provided the output neurons are sigmoid neurons. To see why, consider that when we're setting up the network we usually initialize the weights and biases using some sort of randomization. It may

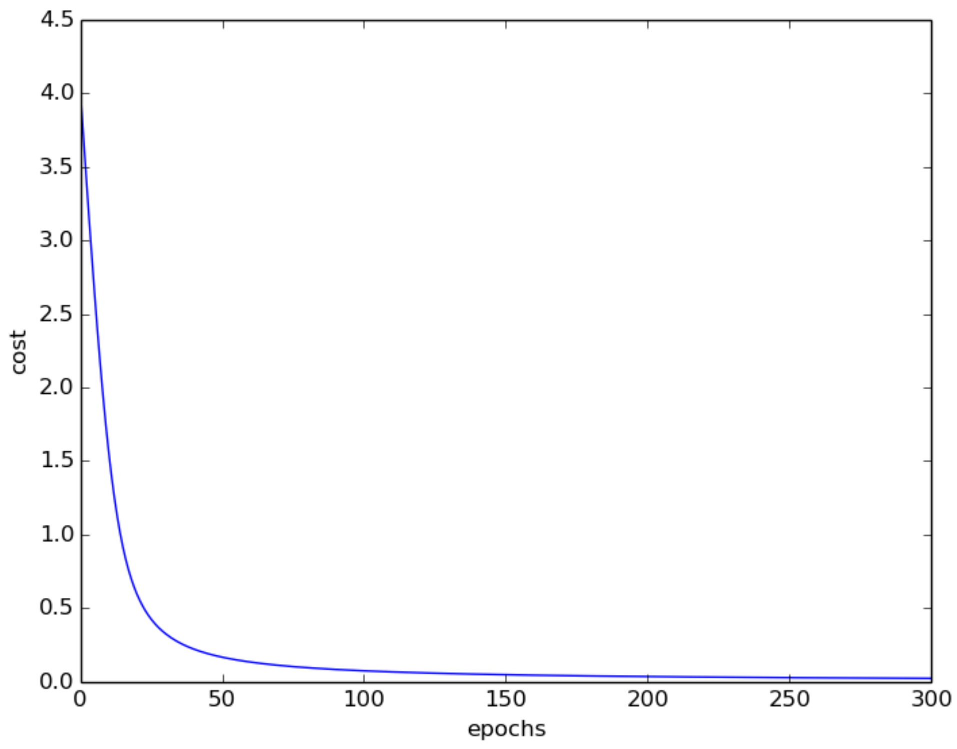


Figure 23: Single neuron with cross entropy cost with weight=2.0, bias=2.0

happen that those initial choices result in the network being decisively wrong for some training input - that is, an output neuron will have saturated near 1, when it should be 0, or vice versa. If we're using the quadratic cost that will slow down learning.

3.3. Softmax

The idea of softmax is to define a new type of output layer for our neural networks. It begins in the same way as with a sigmoid layer, by forming the weighted inputs as $z_j^L = \sum_k w_{jk}^L a^{L-1} \sum_k + b_j^L$. However, in a softmax layer we apply the so-called softmax function to the z_j^L. According to this function, the activation a_j^L of the j^{th} output neuron is

$$a_j^L = \frac{e^{z_j^L}}{\sum_k e^{z_k^L}} \tag{36}$$

where in the denominator we sum over all the output neurons.

To better understand Equation (36), suppose we have a network with four output neurons, and four corresponding weighted inputs, which we'll denote z_1^L, z_2^L, z_3^L and z_4^L. As you increase z_4^L, you'll see an increase in the corresponding output activation, a_4^L, and a decrease in the other output activations. Similarly, if you decrease z_4^L then a_4^L will decrease, and all the other output activations will increase.

In fact, if you look closely, you'll see that in both cases the total change in the other activations exactly compensates for the change in a_4^L. The reason is that the output activations are guaranteed to always sum up to 1,

$$\sum_j a_j^L = \frac{\sum_j e^{z_j^L}}{\sum_k e^{z_k^L}} = 1 \tag{37}$$

And, of course, similar statements hold for all the other activations.

Equation (37) implies that the output from the softmax layer is a set of positive numbers which sum up to 1. In other words, the output from the softmax layer can be thought of as a probability distribution.

In many problems it's convenient to be able to interpret the output activation a_j^L as the network's estimate of the probability that the correct output is j. So, for instance, in the MNIST classification problem, we can interpret a_j^L as the network's estimated probability that the correct digit classification is j.

The learning slowdown problem: How a softmax layer lets us address the learning slowdown problem? To understand that, let's define the log-likelihood cost function. We'll use x to denote a training input to the network, and y to denote the corresponding desired output. Then the log-likelihood cost associated to this training input is

$$C \equiv \ln a_y^L \tag{38}$$

So, for instance, if we're training with MNIST images, and input an image of a 7, then the log-likelihood cost is $\ln a_7^L$. To see that this makes intuitive sense, consider the case when the network is doing a good job, that is, it is confident the input is a 7. In that case it will estimate a value for the corresponding probability a_7^L which is close to 1, and so the cost $\ln a_7^L$ will be small. By contrast, when the network isn't doing such a good job, the probability a_7^L will be smaller, and the cost $\ln a_7^L$ will be larger. Unlike quadratic cost function and cross-entropy function, no need to sum all the cost in the output neurons, only corresponding neuron must be considered. Because the cost of output neurons are related each other to make $\sum_j a_j^L = 1$.

What about the learning slowdown problem? With a little algebra you can show that.

$$\begin{aligned} \frac{\partial C}{\partial b_j^L} &= a_j^L - y_j \\ \frac{\partial C}{\partial w_{jk}^L} &= a_k^{L-1}(a_j^L - y_j) \end{aligned} \tag{39}$$

Here we used y to denote the desired output from the network - e.g., output a "7" if an image of a 7 was input. But in the equations here y to denote the vector of output activations which corresponds to 7, that is, a vector which is all 0 s, except for a 1 in the 7^{th} location.

Just as in the earlier analysis, these expressions ensure that we will not encounter a learning slowdown. In fact, it's useful to think of a softmax output layer with log-likelihood cost as being quite similar to a sigmoid output layer with cross-entropy cost.

3.4. Overfitting

Overfitting is a major problem in neural networks. This is especially true in modern networks, which often have very large numbers of weights and biases.

Let's sharpen this problem up by constructing a situation where our network does a bad job generalizing to new situations. We'll use our 30 hidden neuron network, with its 23,860 parameters. But we won't train the network using all 50,000 MNIST training images. Instead, we'll use just the first 1,000 training images. Using that restricted set will make the problem with generalization much more evident. We'll train in a similar way to before, using the cross-entropy cost function, with a learning rate of $\eta = 0.5$ and a mini-batch size of 10. However, we'll train for 400 epochs, a somewhat larger number than before, because we're not using as many training examples. Get network2.py from https://github.com/mnielsen/neural-networks-and-deep-learning to look at the way the cost function changes:

```
>>> import mnist_loader
>>> training_data, validation_data, test_data = \
mnist_loader.load_data_wrapper()
>>> import network2
>>> net = network2.Network([784, 30, 10], \
                           cost=network2.CrossEntropyCost)
>>> net.large_weight_initializer()
>>> net.SGD(training_data[:1000], 400, 10, 0.5, \
evaluation_data=test_data, \
monitor_evaluation_accuracy=True, \
monitor_training_cost=True)
```

Using the results we can plot the way the cost changes as the network learns.

This looks encouraging, showing a smooth decrease in the cost, just as we expect. Let's now look at how the classification accuracy on the test data changes over time:

If we just look at that cost, it appears that our model is still getting "better". But the test accuracy results show the improvement is an illusion. What our network learns after epoch 280 no longer generalizes to the test data. And so it's not useful learning. We say the network is overfitting or overtraining beyond epoch 280.

Another sign of overfitting may be seen in the classification accuracy on the training data:

The accuracy rises all the way up to 100 percent. That is, our network correctly classifies all 1,000 training images! Meanwhile, our test accuracy tops out at just 82.27 percent. So our network really is learning about peculiarities of the training

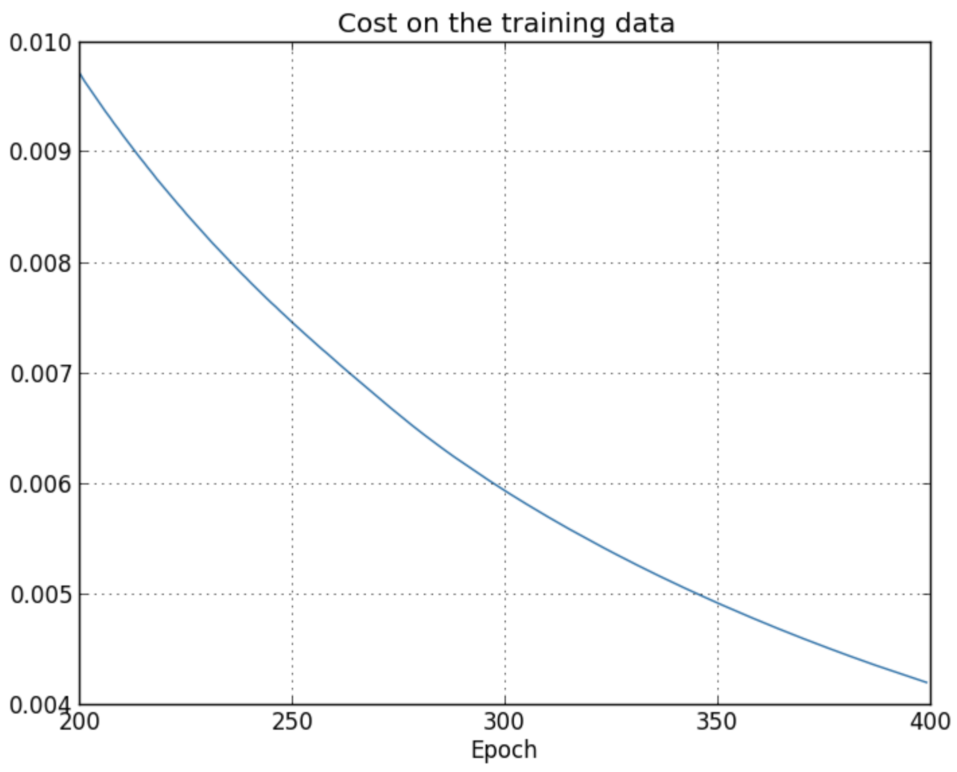


Figure 24: Overfitting effect on the cost of training data

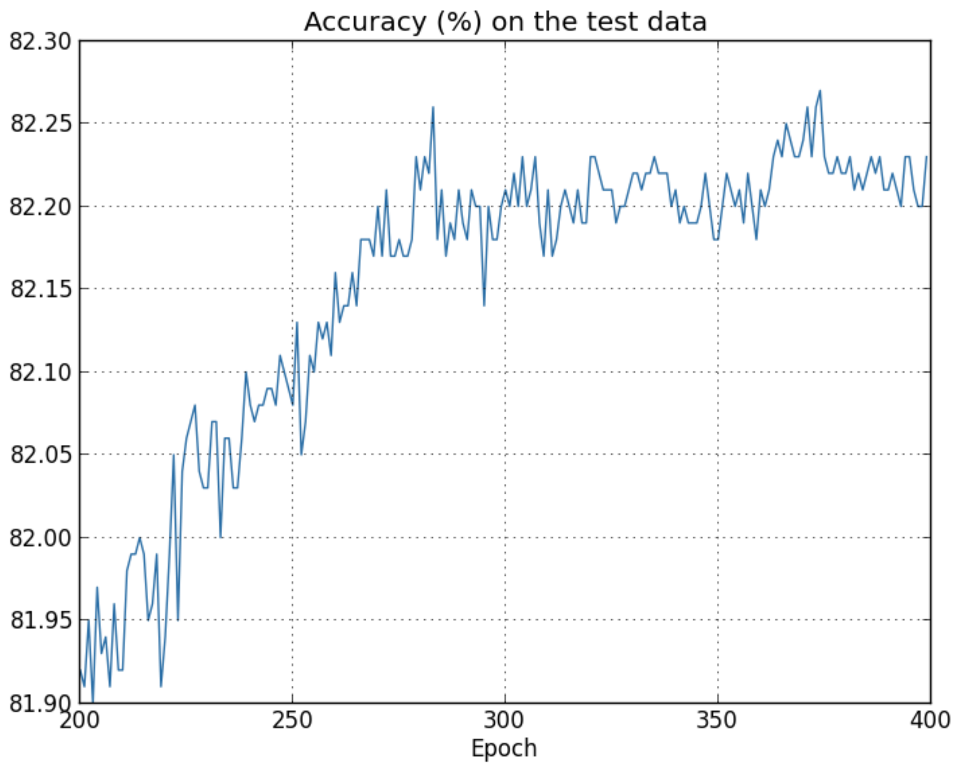


Figure 25: Overfitting effect on the accuracy of test data

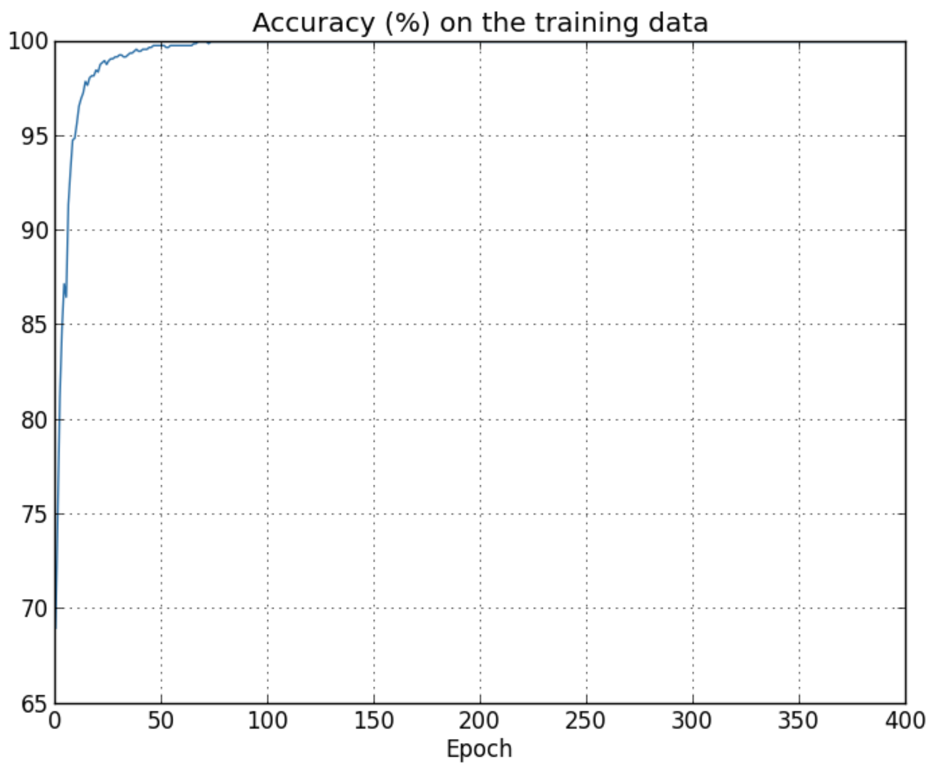


Figure 26: Overfitting effect on the accuracy of training data

set, not just recognizing digits in general. It's almost as though our network is merely memorizing the training set, without understanding digits well enough to generalize to the test set.

The obvious way to detect overfitting is to use the approach above, keeping track of accuracy on the test data as our network trains. If we see that the accuracy on the test data is no longer improving, then we should stop training. Of course, strictly speaking, this is not necessarily a sign of overfitting. It might be that accuracy on the test data and the training data both stop improving at the same time. Still, adopting this strategy will prevent overfitting.

In fact, we'll use a variation on this strategy. Recall that when we load in the MNIST data we load in three data sets:

```
>>> import mnist_loader
>>> training_data, validation_data, test_data = \
mnist_loader.load_data_wrapper()
```

Up to now we've been using the 'training data' and 'test data', and ignoring the 'validation data'. The 'validation data' contains 10,000 images of digits, images which are different from the 50,000 images in the MNIST training set, and the 10,000 images in the MNIST test set.

Instead of using the 'test data' to prevent overfitting, we will use the 'validation data'. To do this, we'll use much the same strategy as was described above for the ‘test data’. That is, we’ll compute the classification accuracy on the ‘validation data’ at the end of each epoch. Once the classification accuracy on the ‘validation data’ has saturated, we stop training. This strategy is called early stopping. Of course, in practice we won’t immediately know when the accuracy has saturated. Instead, we continue training until we’re confident that the accuracy has saturated. It requires some judgement to determine when to stop.

You can think of the validation data as a type of training data that helps us learn good hyper-parameters. This approach to finding good hyper-parameters is sometimes known as the hold out method, since the ‘validation data’ is kept apart from the ‘training data’.

What happens when we use the full training set of 50,000 images? Here’s a graph showing the results for the classification accuracy on both the training data and the test data.

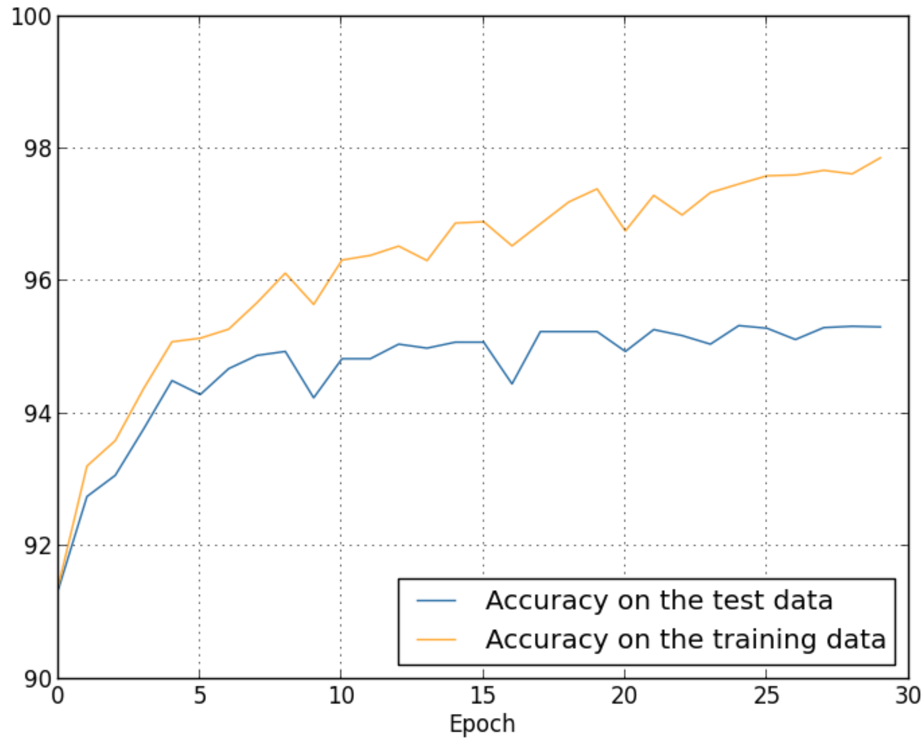


Figure 27: Comparison of accuracies in training and test data

As you can see, the accuracy on the test and training data remain much closer together than when we were using 1,000 training examples. Overfitting is still going on, but it’s been greatly reduced. Our network is generalizing much better from the training data to the test data. In general, one of the best ways of reducing overfitting is to increase the size of the training data. Unfortunately, training data can be expensive or difficult to acquire, so this is not always a practical option.

3.5. Regularization

Fortunately, there are other techniques which can reduce overfitting, even when we have a fixed network and fixed training data. These are known as regularization techniques. One of the most commonly used regularization techniques are weight decay or L2 regularization. The idea of L2 regularization is to add an extra term to the cost function, a term called the regularization term. Here's the regularized cross-entropy:

$$C = -\frac{1}{n}\sum_{xj}\left[y_j \ln a_j^L + (1-y_j)\ln(1-a_j^L)\right] + \frac{\lambda}{2n}\sum_w w^2 \tag{40}$$

The first term is just the usual expression for the cross-entropy. But we've added a second term, namely the sum of the squares of all the weights in the network. This is scaled by a factor $\lambda/2n$, where $\lambda > 0$ is known as the regularization parameter, and n is, as usual, the size of our training set.

Of course, it's possible to regularize other cost functions, such as the quadratic cost. This can be done in a similar way:

$$C = -\frac{1}{2n}\sum_x ||y - a^L||^2 + \frac{\lambda}{2n}\sum_w w^2 \tag{41}$$

Intuitively, the effect of regularization is to make it so the network prefers to learn small weights, all other things being equal. Large weights will only be allowed if they considerably improve the first part of the cost function. Regularization can be viewed as a way of compromising between finding small weights and minimizing the original cost function. When λ is small we prefer to minimize the original cost function, but when λ is large we prefer small weights.

To construct such an example, we first need to figure out how to apply our stochastic gradient descent learning algorithm in a regularized neural network. In particular, we need to know how to compute the partial derivatives $\partial C/\partial w$ and $\partial C/\partial b$ for all the weights and biases in the network.

$$\begin{aligned}\frac{\partial C}{\partial w} &= \frac{\partial C_0}{\partial w} + \frac{\lambda}{n}w \\ \frac{\partial C}{\partial b} &= \frac{\partial C_0}{\partial b}\end{aligned} \tag{42}$$

The $\partial C_0/\partial w$ and $\partial C_0/\partial b$ terms can be computed using backpropagation. Then add $\frac{\lambda}{n}w$ to the partial derivative of all the weight terms. The partial derivatives with respect to the biases are unchanged, and so the gradient descent learning rule for the biases doesn't change from the usual rule:

$$b \rightarrow b\eta\frac{\partial C_0}{\partial b} \tag{43}$$

The learning rule for the weights becomes:

$$\begin{aligned} w &\rightarrow w\eta \frac{\partial C_0}{\partial w} - \frac{\eta\lambda}{n} w \\ &= \left(1 - \frac{\eta\lambda}{n}\right) w - \eta \frac{\partial C_0}{\partial w} \end{aligned} \tag{44}$$

This is exactly the same as the usual gradient descent learning rule, except we first rescale the weight w by a factor $1 - \frac{\eta\lambda}{n}$. This rescaling is sometimes referred to as weight decay, since it makes the weights smaller. At first glance it looks as though this means the weights are being driven unstoppably toward zero. But that's not right, since the other term may lead the weights to increase.

For stochastic gradient descent Equation (43) becomes

$$b \rightarrow b - \frac{\eta}{m} \sum_x \frac{\partial C_x}{\partial b} \tag{45}$$

Equation (44) becomes

$$w \rightarrow \left(1 - \frac{\eta\lambda}{n}\right) w - \frac{\eta}{m} \sum_x \frac{\partial C_x}{\partial w} \tag{46}$$

where the sum is over training examples x in the mini-batch, and C_x is the (unregularized) cost for each training example. And

Let's see how regularization changes the performance of our neural network. We'll use a network with 30 hidden neurons, a mini-batch size of 10, a learning rate of 0.5, and the cross-entropy cost function. However, this time we'll use a regularization parameter of $\lambda = 0.1$.

```
>>> import mnist_loader
>>> training_data, validation_data, test_data =
mnist_loader.load_data_wrapper()
>>> import network2
>>> net = network2.Network([784, 30, 10],
cost=network2.CrossEntropyCost)
>>> net.large_weight_initializer()
>>> net.SGD(training_data[:1000], 400, 10, 0.5,
evaluation_data=test_data, lmbda = 0.1,
monitor_evaluation_cost=True,
monitor_evaluation_accuracy=True,
monitor_training_cost=True,
monitor_training_accuracy=True)
```

The cost on the training data decreases over the whole time, much as it did in the earlier, unregularized case.

But this time the accuracy on the 'test data' continues to increase for the entire 400 epochs:

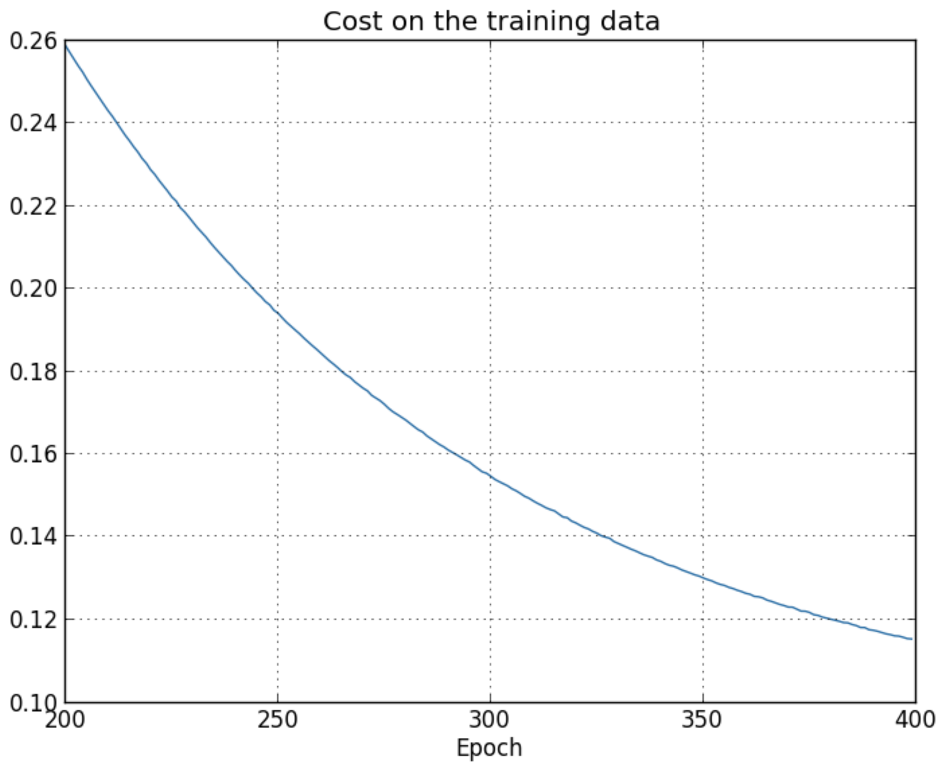


Figure 28: Cost in training data for regularized case

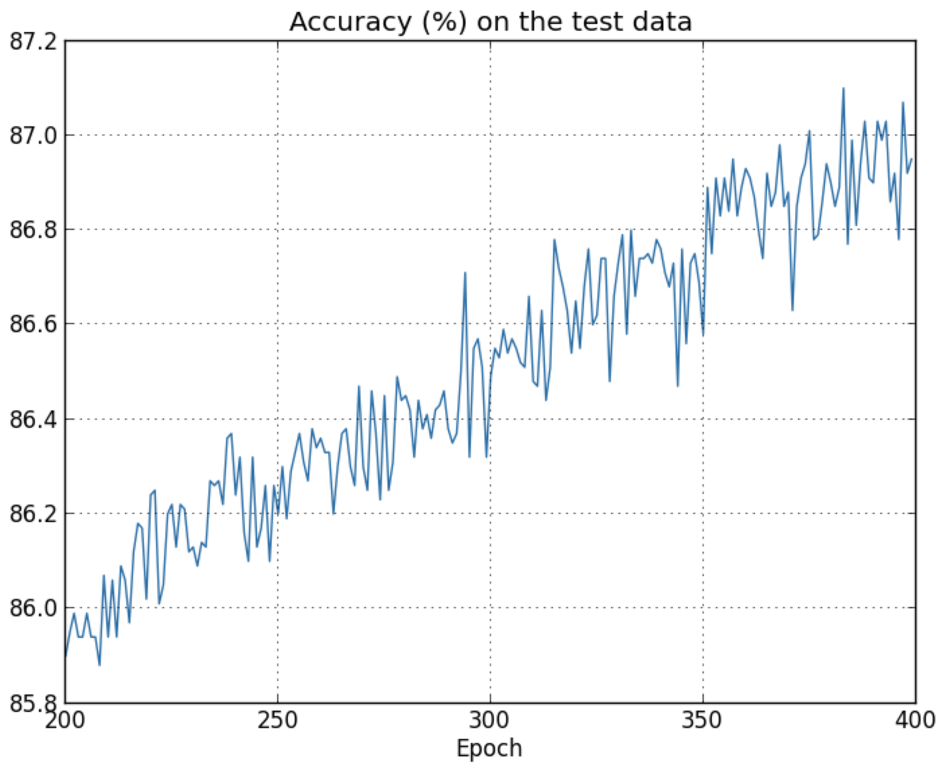


Figure 29: Accuracy in test data for regularized case

Clearly, the use of regularization has suppressed overfitting. What's more, the accuracy is considerably higher, with a peak classification accuracy of 87.1 percent, compared to the peak of 82.27 percent obtained in the unregularized case. It seems that, empirically, regularization is causing our network to generalize better, and considerably reducing the effects of overfitting.

Let' train our network with full 50,000 images. The hyper-parameters the same as before - 30 epochs, learning rate 0.5, mini-batch size of 10. However, we need to modify the regularization parameter. The reason is because the size n of the training set has changed from $n = 1,000$ to $n = 50,000$. If we continued to use $\lambda = 0.1$ that would mean much less weight decay, and thus much less of a regularization effect. We compensate by changing to $\lambda = 5.0$.

```
>>> net.large_weight_initializer()
>>> net.SGD(training_data, 30, 10, 0.5,
evaluation_data=test_data, lmbda = 5.0,
monitor_evaluation_accuracy=True,
monitor_training_accuracy=True)
```

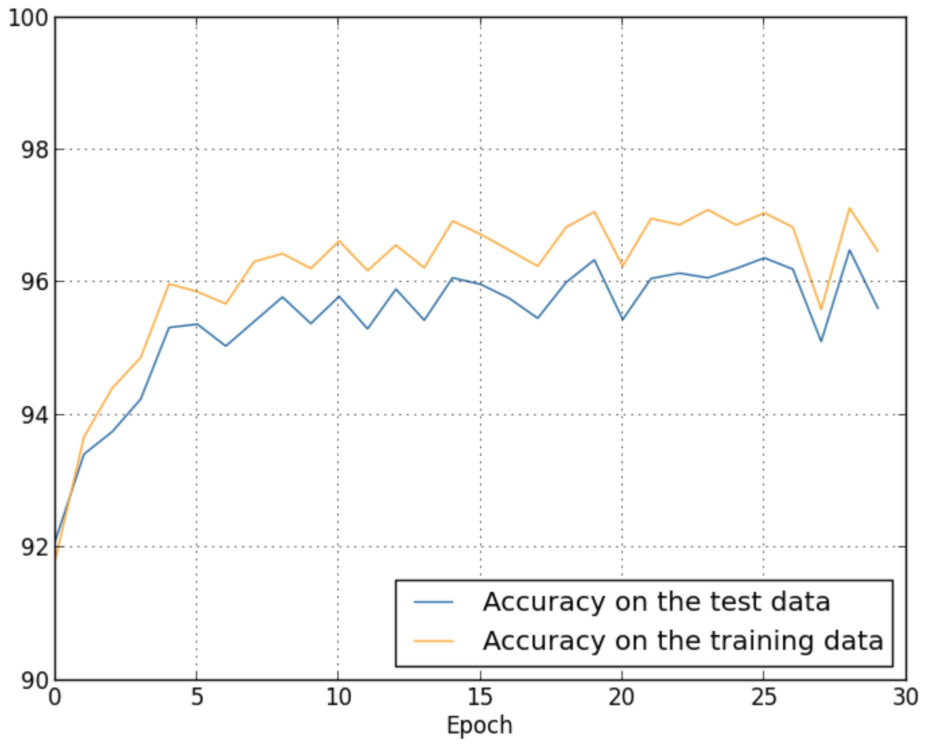


Figure 30: Comparison of accuracies of training and test data

There's lots of good news here. First, our classification accuracy on the test data is up, from 95.49 percent when running unregularized, to 96.49 percent. That's a big improvement. Second, we can see that the gap between results on the training and test data is much narrower than before, running at under a percent. That's still a significant gap, but we've obviously made substantial progress reducing overfitting.

Finally, let's see what test classification accuracy we get when we use 100 hidden neurons and a regularization parameter of $\lambda = 5.0$.

```
>>> net = network2.Network([784, 100, 10],
cost=network2.CrossEntropyCost)
>>> net.large_weight_initializer()
>>> net.SGD(training_data, 30, 10, 0.5, lmbda=5.0,
evaluation_data=validation_data,
monitor_evaluation_accuracy=True)
```

The final result is a classification accuracy of 97.92 percent on the validation data.

Empirically, when doing multiple runs of our MNIST networks, but with different (random) weight initializations, I've found that the unregularized runs will occasionally get "stuck", apparently caught in local minima of the cost function. By contrast, the regularized runs have provided much more easily replicable results.

Heuristically, if the cost function is unregularized, then the length of the weight vector is likely to grow, all other things being equal. Over time this can lead to the weight vector being very large indeed and can cause the weight vector to get stuck pointing in more or less the same direction, since changes due to gradient descent only make tiny changes to the direction.

3.5.1. Other techniques for regularization

There are three other approaches to reducing overfitting: L1 regularization, dropout, and artificially expanding the training set size.

3.5.1.1. L1 regularization

In this approach we modify the unregularized cost function by adding the sum of the absolute values of the weights:

$$C = C_0 + \frac{\lambda}{n} \sum_w |w| \tag{47}$$

Intuitively, this is similar to L2 regularization, penalizing large weights, and tending to make the network prefer small weights.

To do that, we'll look at the partial derivatives of the cost function. Differentiating (47) we obtain:

$$\frac{\partial C}{\partial w} = \frac{\partial C_0}{\partial w} + \frac{\lambda}{n} \operatorname{sgn}(w) \tag{48}$$

where $\operatorname{sgn}(w)$ is the sign of w, that is, $+1$ if w is positive, and -1 if w is negative. The resulting update rule for an L1 regularized network is

$$w \to w\frac{\eta\lambda}{n}\operatorname{sgn}(w) - \eta\frac{\partial C_0}{\partial w} \tag{49}$$

In both expressions the effect of regularization is to shrink the weights. This accords with our intuition that both kinds of regularization penalize large weights. But the way the weights shrink is different. In L1 regularization, the weights shrink by a constant amount toward 0. In L2 regularization, the weights shrink by an amount which is proportional to w. And so when a particular weight has a large magnitude, $|w|$, L1 regularization shrinks the weight much less than L2 regularization does. By contrast, when $|w|$ is small, L1 regularization shrinks the weight much more than L2 regularization. The net result is that L1 regularization tends to concentrate the weight of the network in a relatively small number of high-importance connections, while the other weights are driven toward zero.

Partial derivative $\partial C/\partial w$ isn't defined when $w = 0$. The reason is that the function $|w|$ has a sharp "corner" at $w = 0$, and so isn't differentiable at that point. That's okay, though. We'll use Equations (48) and (49) with the convention that $\operatorname{sgn}(0) = 0$.

3.5.1.2. Dropout

Dropout is a radically different technique for regularization. In dropout we modify the network itself. Suppose we're trying to train a network:

With dropout, we start by randomly (and temporarily) deleting half the hidden neurons in the network, while leaving the input and output neurons untouched. After doing this, we'll end up with a network along the following lines.

After doing this over a mini-batch of examples, we update the appropriate weights and biases. We then repeat the process, first restoring the dropout neurons, then choosing a new random subset of hidden neurons to delete, estimating the gradient for a different mini-batch, and updating the weights and biases in the network.

By repeating this process over and over, our network will learn a set of weights and biases. Of course, those weights and biases will have been learnt under conditions in which half the hidden neurons were dropped out. When we actually run the full network that means that twice as many hidden neurons will be active. To compensate for that, we halve the weights outgoing from the hidden neurons.

Heuristically, when we dropout different sets of neurons, it's rather like we're training different neural networks. And so the dropout procedure is like averaging the effects of a very large number of different networks. The different networks will overfit in different ways, and so, hopefully, the net effect of dropout will be to reduce overfitting.

In other words, if we think of our network as a model which is making predictions, then we can think of dropout as a way of making sure that the model is robust to the loss of any individual piece of evidence.

Here some dropout results applied on MNIST data set.

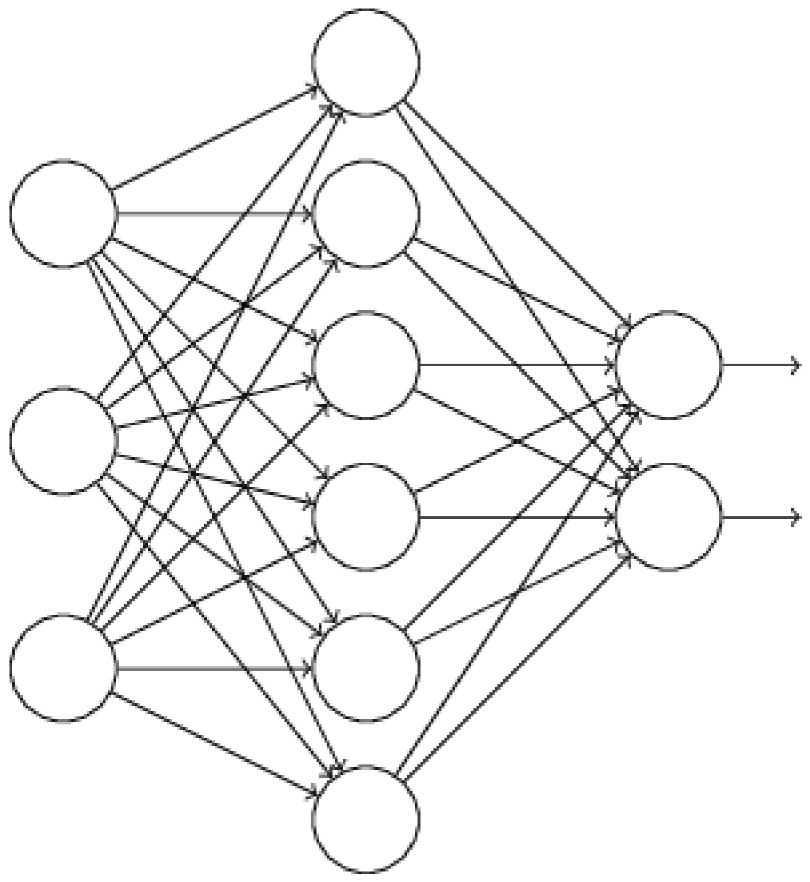


Figure 31: MLP

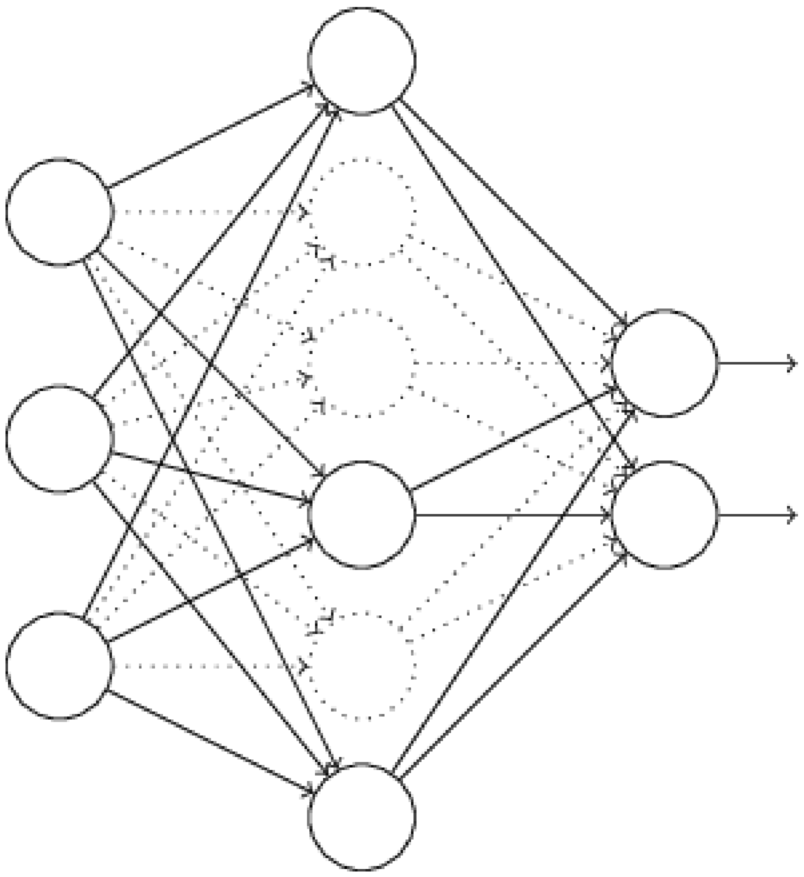


Figure 32: Dropping neurons out

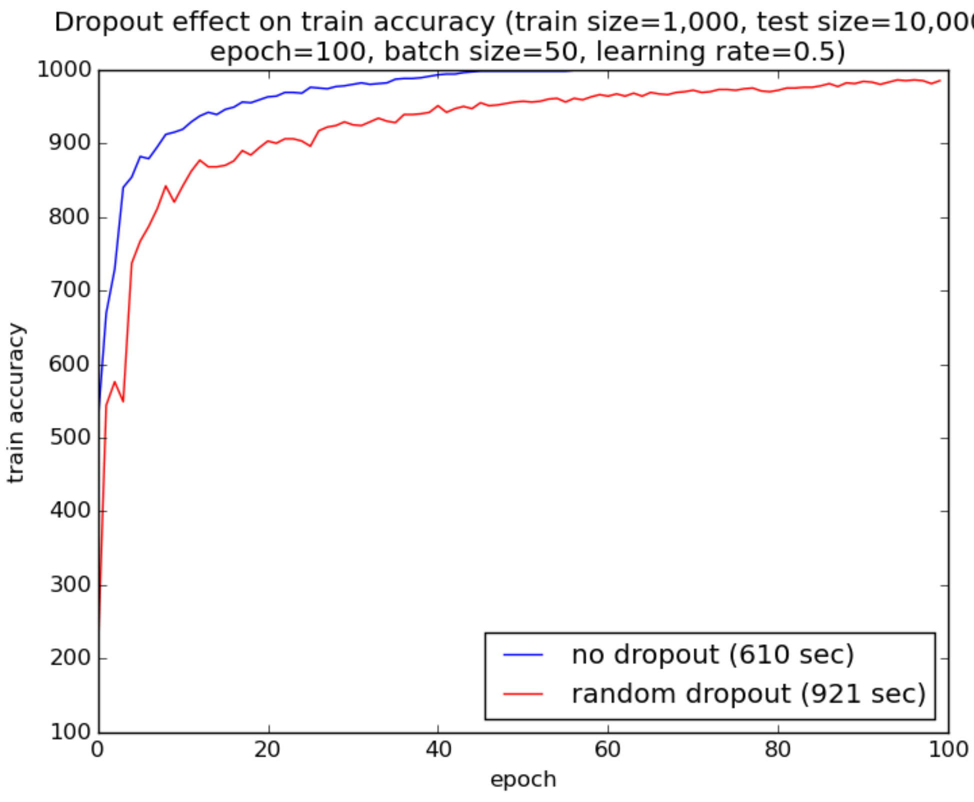


Figure 33: Dropout effect on train accuracy

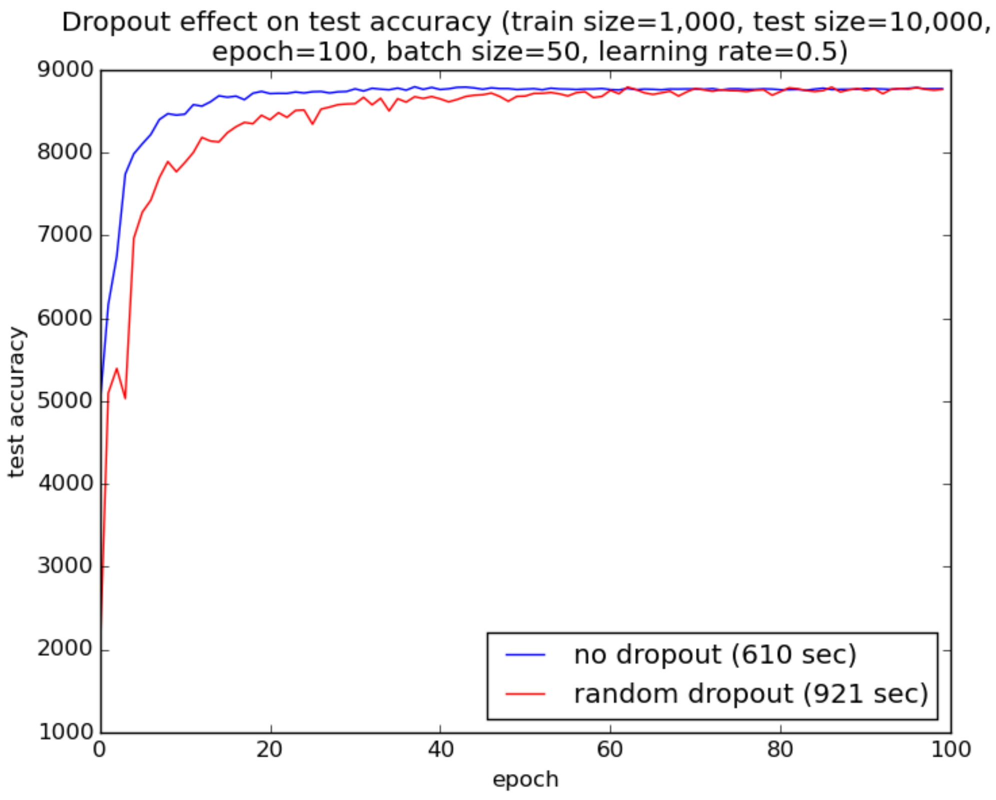


Figure 34: Dropout effect on test accuracy

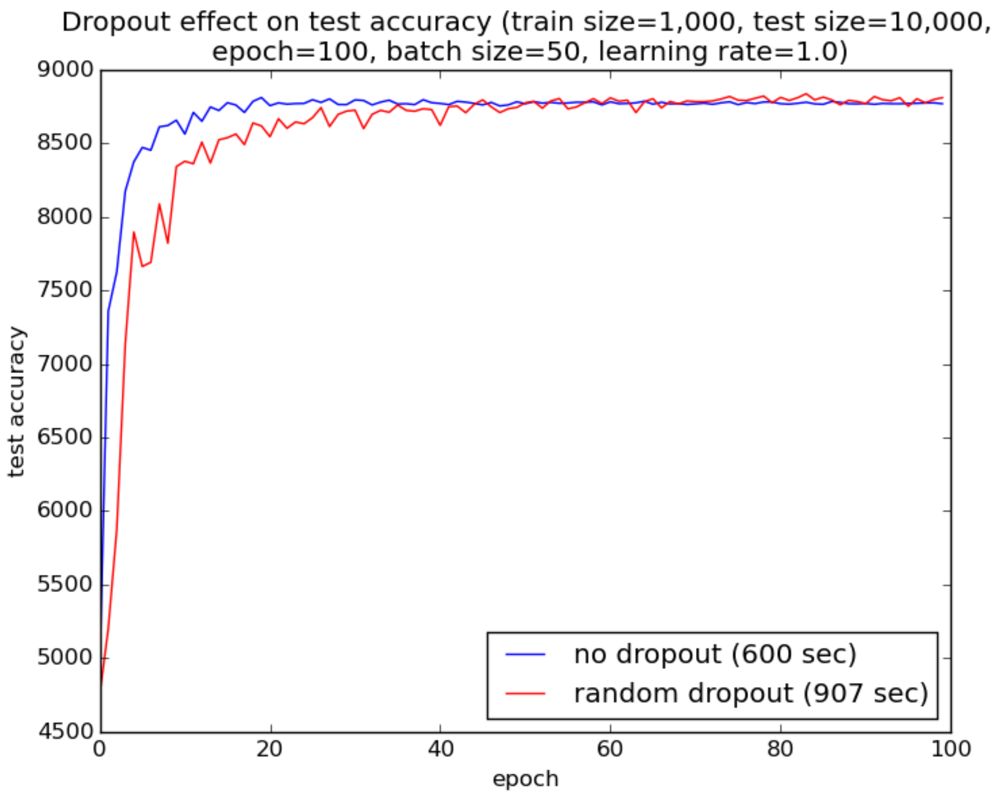


Figure 35: Dropout effect on test accuracy

3.6. Artificially expanding the training data

Obtaining more training data is a great idea. Unfortunately, it can be expensive, and so is not always possible in practice. However, there's another idea which can work nearly as well, and that's to artificially expand the training data. Suppose, for example, that we take an MNIST training image of a five,

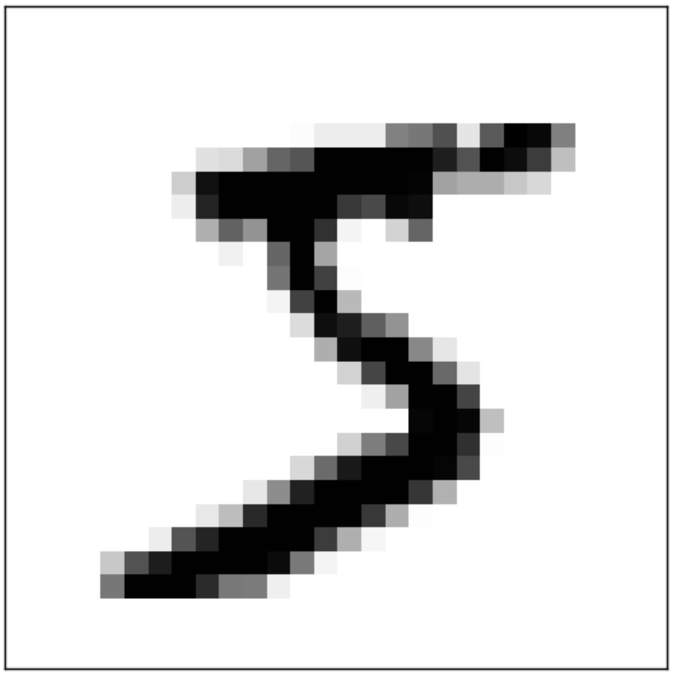


Figure 36: Normal number five

and rotate it by a small amount, let's say 15 degrees:

It's still recognizably the same digit. And yet at the pixel level it's quite different to any image currently in the MNIST training data. It's conceivable that adding this image to the training data might help our network learn more about how to classify digits. Also we can expand our training data by making many small rotations of all the MNIST training images, and then using the expanded training data to improve our network's performance.

3.7. How to choose a neural network's hyper-parameters?

3.7.1. Broad strategy

Suppose, for example, that you're attacking MNIST for the first time. You start out enthusiastic, but are a little discouraged when your first network fails completely, as in the example above. The way to go is to strip the problem down. Get rid of all the training and validation images except images which are 0s or

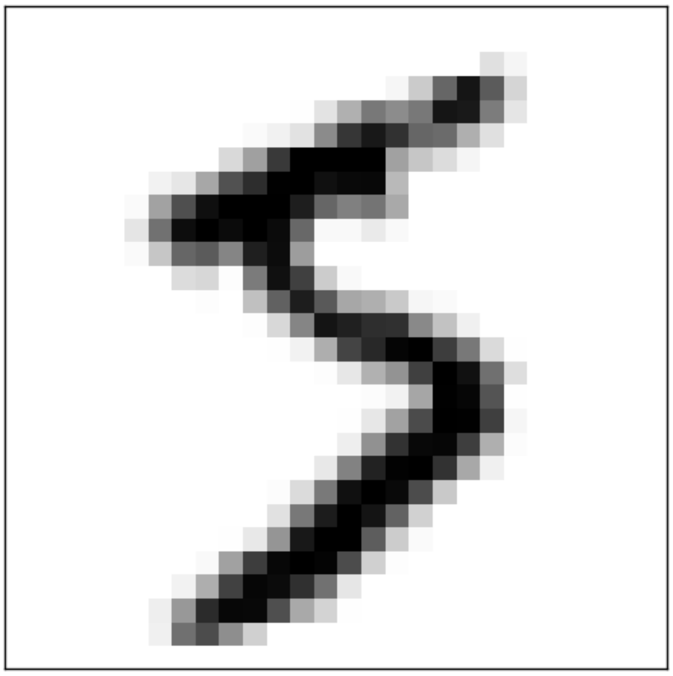


Figure 37: Rotated number five

1s. Then try to train a network to distinguish 0s from 1s. Not only is that an inherently easier problem than distinguishing all ten digits, it also reduces the amount of training data by 80 percent, speeding up training by a factor of 5. That enables much more rapid experimentation, and so gives you more rapid insight into how to build a good network.

You can further speed up experimentation by stripping your network down to the simplest network likely to do meaningful learning. If you believe a [784, 10] network can likely do better-than-chance classification of MNIST digits, then begin your experimentation with such a network. It'll be much faster than training a [784, 30, 10] network, and you can build back up to the latter.

You can get another speed up in experimentation by increasing the frequency of monitoring. Of course, a minute isn't really very long to wait for all training, but if you want to trial dozens of hyper-parameter choices it's annoying. We can get feedback more quickly by monitoring the validation accuracy more often, say, after every 1,000 training images. Furthermore, instead of using the full 10,000 image validation set to monitor performance, we can get a much faster estimate using just 100 validation images.

And so we can continue, individually adjusting each hyper-parameter, gradually improving performance. Once we've explored to find an improved value for η, then we move on to find a good value for λ. Then experiment with a more complex architecture, say a network with 10 hidden neurons. Then adjust the values for η and λ again. Then increase to 20 hidden neurons. And then adjust other hyper-parameters some more.

3.7.2. Learning rate

Suppose we run three MNIST networks with three different learning rates, $\eta = 0.025$, $\eta = 0.25$ and $\eta = 2.5$, respectively. Here's a graph showing the behaviour of the training cost as we train.

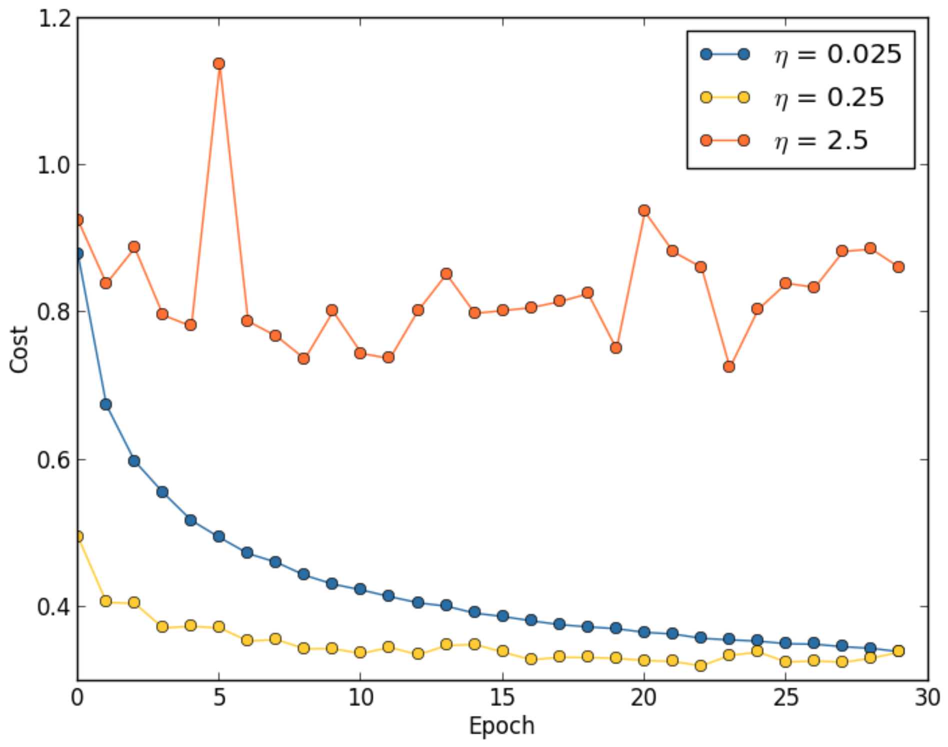


Figure 38: Comparison of learning rates

With $\eta = 0.025$ the cost decreases smoothly until the final epoch. With $\eta = 0.25$ the cost initially decreases, but after about 20 epochs it is near saturation, and thereafter most of the changes are merely small and apparently random oscillations. Finally, with $\eta = 2.5$ the cost makes large oscillations right from the start.

Of course, choosing η so small creates another problem, namely, that it slows down stochastic gradient descent. An even better approach would be to start with $\eta = 0.25$, train for 20 epochs, and then switch to $\eta = 0.025$. We'll discuss such variable learning rate schedules later.

With this picture in mind, we can set η as follows. First, we estimate the threshold value for η at which the cost on the training data immediately begins decreasing, instead of oscillating or increasing. This estimate doesn't need to be too accurate. You can estimate the order of magnitude by starting with $\eta = 0.01$. If the cost decreases during the first few epochs, then you should successively try $\eta = 0.1, 1.0, \ldots$ until you find a value for η where the cost oscillates or increases during the first few epochs. Alternately, if the cost oscillates or increases during the first few epochs when $\eta = 0.01$, then try $\eta = 0.001, 0.0001, \ldots$ until you find a value for η where the cost decreases during the first few epochs.

3.7.3. Use early stopping to determine the number of training epochs

As we discussed earlier in the chapter, early stopping means that at the end of each epoch we should compute the classification accuracy on the validation data. When that stops improving, terminate. This makes setting the number of epochs very simple. Furthermore, early stopping also automatically prevents us from overfitting.

3.7.4. Learning rate schedule

We've been holding the learning rate η constant. However, it's often advantageous to vary the learning rate. Early on during the learning process it's likely that the weights are badly wrong. And so it's best to use a large learning rate that causes the weights to change quickly.

How should we set our learning rate schedule? Many approaches are possible. The idea is to hold the learning rate constant until the validation accuracy starts to get worse. Then decrease the learning rate by some amount, say a factor of two or ten. We repeat this many times, until, say, the learning rate is a factor of 1,024 (or 1,000) times lower than the initial value. Then we terminate.

3.7.5. The regularization parameter

The suggestion is starting initially with no regularization $\lambda = 0.0$, and determining a value for η, as above. Using that choice of η, we can then use the validation data to select a good value for λ. Start by trialling let' s say $\lambda = 1.0$ and then increase or decrease by factors of 10, as needed to improve performance on the validation data.

3.7.6. Mini-batch size

Let' s first suppose that we're doing online learning, i.e., that we're using a mini-batch size of 1.

The obvious worry about online learning is that using mini-batches which contain just a single training example will cause significant errors in our estimate of the gradient. In fact, though, the errors turn out to not be such a problem. The reason is that the individual gradient estimates don't need to be super-accurate. All we need is an estimate accurate enough that our cost function tends to keep decreasing.

Summing up: Keep in mind that the heuristics described here are rules of thumb, not rules cast in stone. You should be on the lookout for signs that things aren't working, and be willing to experiment.

One thing that becomes clear as you read these articles and, especially, as you engage in your own experiments, is that hyper-parameter optimization is not a problem that is ever completely solved. There's always another trick you can try to improve performance.

3.8. Other techniques

3.8.1. Hessian technique To begin our discussion it helps to put neural networks aside for a bit. Instead, we're just going to consider the abstract problem of minimizing a cost function C which is a function of many variables, $w = w_1, w_2, \ldots,$ so $C = C(w)$. By Taylor's theorem, the cost function can be approximated near a point w by

$$\begin{aligned} C(w + \Delta w) = C(w) &+ \sum_j \frac{\partial C}{\partial w_j} \Delta w_j \\ &+ \frac{1}{2} \sum_{jk} \Delta w_j \frac{\partial^2 C}{\partial w_j \partial w_k} \Delta w_k + \ldots \end{aligned} \tag{50}$$

We can rewrite this more compactly as

$$C(w + \Delta w) = C(w) + \nabla C \cdot \Delta w + \frac{1}{2} \Delta w^T H \Delta w + \tag{51}$$

where ∇C is the usual gradient vector, and H is a matrix known as the Hessian matrix, whose jk^{th} entry is $\partial^2 C / \partial w_j \partial w_k$. Suppose we approximate C by discarding the higher-order terms represented by $\ldots$ above,

$$C(w + \Delta w) \approx C(w) + \nabla C \cdot \Delta w + \frac{1}{2} \Delta w^T H \Delta w \tag{52}$$

Using calculus we can show that the expression on the right-hand side can be minimized by choosing

$$\Delta w = H^1 \nabla C \tag{53}$$

In practice, (53) is only an approximation, and it's better to take smaller steps. We do this by repeatedly changing w by an amount $\Delta w = -\eta H^1 \nabla C$, where η is known as the learning rate.

This approach to minimizing a cost function is known as the Hessian technique or Hessian optimization. There are theoretical and empirical results showing that Hessian methods converge on a minimum in fewer steps than standard gradient descent. In particular, by incorporating information about second-order changes in the cost function it's possible for the Hessian approach to avoid many pathologies that can occur in gradient descent. Furthermore, there are versions of the backpropagation algorithm which can be used to compute the Hessian.

Unfortunately, while it has many desirable properties, it has one very undesirable property: the Hessian matrix is very big. Suppose you have a neural network with 10^7 weights and biases. Then the corresponding Hessian matrix will contain $10^7 \times 10^7 = 10^{14}$ entries. That's a lot of entries to compute, especially when you're going to need to invert the matrix as well! That makes Hessian optimization difficult to apply in practice.

Momentum-based gradient descent Unlike Hessian technique momentum-based gradient descent avoids large matrices of second derivatives. The momentum technique modifies gradient descent in two ways that make it more similar to the physical picture. First, it introduces a notion of "velocity" for the parameters we're trying to optimize. The gradient acts to change the velocity, not (directly) the "position", in much the same way as physical forces change the velocity, and only indirectly affect position. Second, the momentum method introduces a kind of friction term, which tends to gradually reduce the velocity.

We introduce velocity variables $v = v_1, v_2, \dots$ one for each corresponding w_j variable. Then we replace the gradient descent update rule $w \to w = w - \eta \nabla C$ by

$$\begin{aligned} v &\to \mu v - \eta \nabla C \\ w &\to w + v \end{aligned} \tag{54}$$

In these equations, μ is a hyper-parameter which controls the amount of damping or friction in the system. To understand the meaning of the equations it's helpful to first consider the case where $\mu = 1$, which corresponds to no friction. When that's the case, inspection of the equations shows that the "force" ∇C is now modifying the velocity, v, and the velocity is controlling the rate of change of w. Intuitively, we build up the velocity by repeatedly adding gradient terms to it. That means that if the gradient is in (roughly) the same direction through several rounds of learning, we can build up quite a bit of steam moving in that direction. Think, for example, of what happens if we're moving straight down a slope. With each step the velocity gets larger down the slope, so we move more and more quickly to the bottom of the valley. This can enable the momentum technique to work much faster than standard gradient descent. Of course, a problem is that once we reach the bottom of the valley we will overshoot. Or, if the gradient should change rapidly, then we could find ourselves moving in the wrong direction. That's the reason for the μ hyper-parameter in (54). To be a little more precise, you should think of 1μ as the amount of friction in the system. When $\mu = 1$, as we've seen, there is no friction, and the velocity is completely driven by the gradient ∇C. By contrast, when $\mu = 0$ there's a lot of friction, the velocity can't build up, and Equation (54) reduce to the usual equation for gradient descent, $w \to w = w\eta\nabla C$

It' s avoided naming the hyper-parameter μ up to now. The reason is that the standard name for μ is badly chosen: it's called the momentum co-efficient. This is potentially confusing, since μ is not at all the same as the notion of momentum from physics. Rather, it is much more closely related to friction.

A nice thing about the momentum technique is that it takes almost no work to modify an implementation of gradient descent to incorporate momentum. We can still use backpropagation to compute the gradients, just as before, and use ideas such as sampling stochastically chosen mini-batches. In this way, we can get some of the advantages of the Hessian technique, using information about how the gradient is changing. In practice, the momentum technique is commonly used, and often speeds up learning.

Other models of artificial neuron

Up to now we've built our neural networks using sigmoid neurons. In practice, networks built using other model neurons sometimes outperform sigmoid networks.

Perhaps the simplest variation is the tanh (pronounced "tanch") neuron, which replaces the sigmoid function by the hyperbolic tangent function. The output of a tanh neuron with input x, weight vector w, and bias b is given by

$$\tanh(w \cdot x + b) \tag{55}$$

Recall that the tanh function is defined by

$$\tanh(z) \equiv \frac{e^z e^{-z}}{e^z + e^{-z}} \tag{56}$$

With a little algebra it can easily be verified that

$$\sigma(z) = \frac{1 + \tanh(z/2)}{2} \tag{57}$$

that is, tanh is just a rescaled version of the sigmoid function. We can also see graphically that the tanh function has the same shape as the sigmoid function,

One difference between tanh neurons and sigmoid neurons is that the output from tanh neurons ranges from -1 to 1, not 0 to 1. This means that if you're going to build a network based on tanh neurons you may need to normalize your outputs.

If some of the input activations have different signs, replace the sigmoid by an activation function, such as tanh, which allows both positive and negative activations. Indeed, because tanh is symmetric about zero, $\tanh(z) = tanh(z)$.

Another variation on the sigmoid neuron is the rectified linear neuron or rectified linear unit. The output of a rectified linear unit with input x, weight vector w, and bias b is given by

$$\max(0, w \cdot x + b) \tag{58}$$

Graphically, the rectifying function $\max(0, z)$ looks like this:

Like the sigmoid and tanh neurons, rectified linear units can be used to compute any function, and they can be trained using ideas such as backpropagation and stochastic gradient descent.

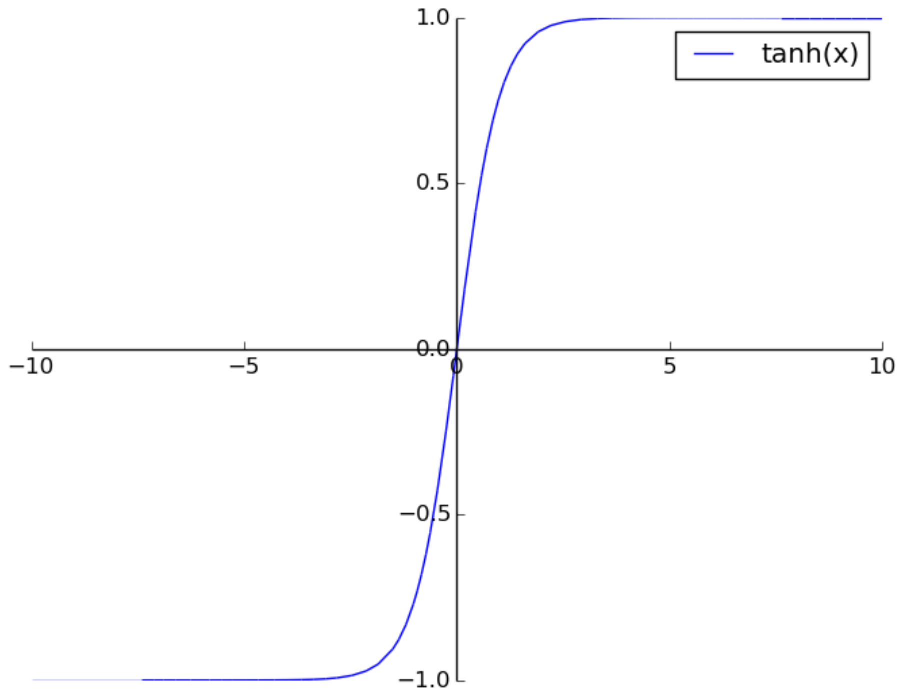


Figure 39: Tanh function

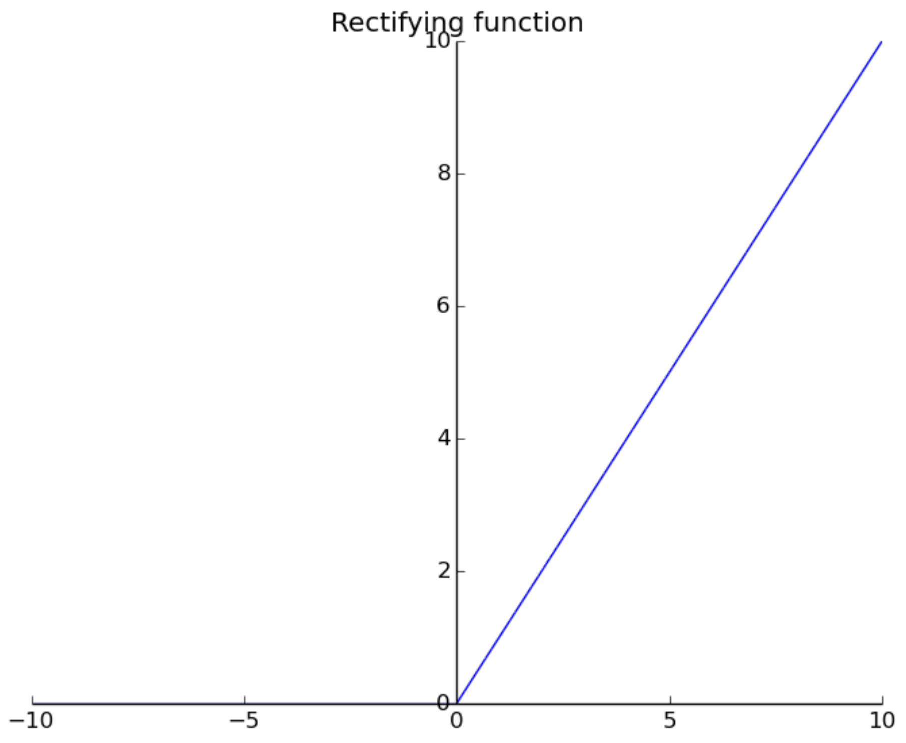


Figure 40: Rectifying function