Neural Networks^{*}

March 15, 2022

1 Introduction

The human visual system is one of the wonders of the world. Consider the following sequence of handwritten digits:

504192

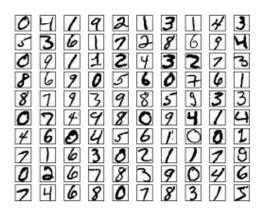
Most people effortlessly recognize those digits as 504192. That ease is deceptive. In each hemisphere of our brain, humans have a primary visual cortex, also known as V_1 , containing 140 million neurons, with tens of billions of connections between them. And yet human vision involves not just V_1 , but an entire series of visual cortices – V_2 , V_3 , V_4 , and V_5 – doing progressively more complex image processing. We carry in our heads a supercomputer, tuned by evolution over hundreds of millions of years, and superbly adapted to understand the visual world. Recognizing handwritten digits isn't easy. Rather, we humans are stupendously, astoundingly good at making sense of what our eyes show us. But nearly all that work is done unconsciously. And so we don't usually appreciate how tough a problem our visual systems solve.

The difficulty of visual pattern recognition becomes apparent if you attempt to write a computer program to recognize digits like those above. What seems easy when we do it ourselves suddenly becomes extremely difficult. Simple intuitions about how we recognize shapes – "a 9 has a loop at the top, and a vertical stroke in the bottom right" – turn out to be not so simple to express algorithmically. When you try to make such rules precise, you quickly get lost in a morass of exceptions and caveats and special cases. It seems hopeless.

Neural networks approach the problem in a different way. The idea is to take a large number of handwritten digits, known as training examples,

^{*}References

⁻ Mickael Nielsen. Neural Networks and Deep Learning



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 hand-written digits. Furthermore, by increasing the number of training examples, the network can learn more about handwriting, and so improve its accuracy. So while I've shown just 100 training digits above, perhaps we could build a better handwriting recognizer by using thousands or even millions or billions of training examples.

In this lecture notes we'll write a computer program implementing a neural network that learns to recognize handwritten digits. The program is just 74 lines long, and uses no special neural network libraries. But this short program can recognize digits with an accuracy over 96 percent, without human intervention. Furthermore, in later lecture notes we'll develop ideas which can improve accuracy to over 99 percent. In fact, the best commercial neural networks are now so good that they are used by banks to process cheques, and by post offices to recognize addresses.

We're focusing on handwriting recognition because it's an excellent prototype problem for learning about neural networks in general. As a prototype it hits a sweet spot: it's challenging – it's no small feat to recognize handwritten digits – but it's not so difficult as to require an extremely complicated solution, or tremendous computational power. Furthermore, it's a great way to develop more advanced techniques, such as deep learning. And so throughout the course we'll return repeatedly to the problem of handwriting recognition. Later in the lecture, we'll discuss how these ideas may be applied to other problems in computer vision, and also in speech, natural language processing, and other domains.

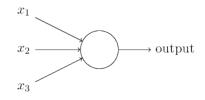
Of course, if the point of the lecture notes was only to write a computer program to recognize handwritten digits, then the lecture notes would be much shorter! But along the way we'll develop many key ideas about neural networks, including two important types of artificial neuron (the perceptron and the sigmoid neuron), and the standard learning algorithm for neural networks, known as stochastic gradient descent. Throughout, I focus on explaining *why* things are done the way they are, and on building your neural networks intuition. That requires a lengthier discussion than if I just presented the basic mechanics of what's going on, but it's worth it for the deeper understanding you'll attain. Amongst the payoffs, by the end of the lecture notes we'll be in position to understand what deep learning is, and why it matters.

2 Perceptrons

What is a neural network? To get started, I'll explain a type of artificial neuron called a *perceptron*. 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*. We'll get to sigmoid neurons shortly. But to understand why sigmoid neurons are defined the way they are, it's worth taking the time to first understand perceptrons.

So how do perceptrons work? A perceptron takes several binary inputs, x_1, x_2, \ldots , and produces a single binary output:



In the example shown the perceptron has three inputs, x_1 , x_2 , x_3 . 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:

$$\text{output} = \begin{cases} 0 & \text{if} \quad \sum_{j} w_{j} x_{j} \leq \text{threshold} \\ 1 & \text{if} \quad \sum_{j} w_{j} x_{j} > \text{threshold} \end{cases}$$
(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. Let me give an example. It's not a very realistic example, but it's easy to understand, and we'll soon get to more realistic examples. Suppose the weekend is coming up, and you've heard that there's going to be a cheese festival in your city. You like cheese, and are trying to decide whether or not to go to the festival. You might make your decision by weighing up three factors:

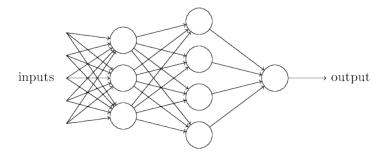
- 1) Is the weather good?
- 2) Does your boyfriend or girlfriend want to accompany you?
- 3) Is the festival near public transit? (You don't own a car).

We can represent these three factors by corresponding binary variables x_1 , x_2 and x_3 . For instance, we'd have $x_1 = 1$ if the weather is good, and $x_1 = 0$ if the weather is bad. Similarly, $x_2 = 1$ if your boyfriend or girlfriend wants to go, and $x_2 = 0$ if not. And similarly again for x_3 and public transit.

Now, suppose you absolutely adore cheese, so much so that you're happy to go to the festival even if your boyfriend or girlfriend is uninterested and the festival is hard to get to. But perhaps you really loathe bad weather, and there's no way you'd go to the festival if the weather is bad. You can use perceptrons to model this kind of decisionmaking. One way to do this is to choose a weight $w_1 = 6$ for the weather, and $w_2 = 2$ and $w_3 = 2$ for the other conditions. The larger value of w_1 indicates that the weather matters a lot to you, much more than whether your boyfriend or girlfriend joins you, or the nearness of public transit. Finally, suppose you choose a threshold of 5 for the perceptron. With these choices, the perceptron implements the desired decision-making model, outputting 1 whenever the weather is good, and 0 whenever the weather is bad. It makes no difference to the output whether your boyfriend or girlfriend wants to go, or whether public transit is nearby.

By varying the weights and the threshold, we can get different models of decisionmaking. For example, suppose we instead chose a threshold of 3. Then the perceptron would decide that you should go to the festival whenever the weather was good or when both the festival was near public transit and your boyfriend or girlfriend was willing to join you. In other words, it'd be a different model of decision-making. Dropping the threshold means you're more willing to go to the festival.

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 – what we'll call 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.

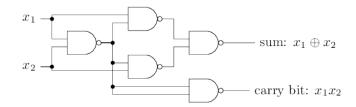
Incidentally, when I defined perceptrons I said that a perceptron has just a single output. In the network above the perceptrons look like they have multiple outputs. In fact, they're still single output. The multiple output arrows are merely a useful way of indicating that the output from a perceptron is being used as the input to several other perceptrons. It's less unwieldy than drawing a single output line which then splits.

Let's simplify the way we describe perceptrons. The condition $\sum_j w_j x_j$ >threshold is cumbersome, and we can make two notational changes to simplify it. The first change is to write $\sum_j w_j x_j$ as a dot product, $w \cdot x = \sum_j w_j x_j$, 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= -threshold. Using the bias instead of the threshold, the perceptron rule can be rewritten:

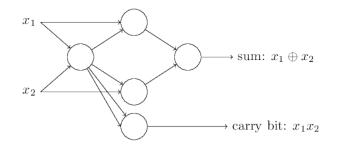
$$output = \begin{cases} 0 & \text{if } w \cdot x + b \le 0\\ 1 & \text{if } w \cdot x + b > 0 \end{cases}$$
(2)

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. Obviously, introducing the bias is only a small change in how we describe perceptrons, but we'll see later that it leads to further notational simplifications. Because of this, in the remainder of the lecture notes we won't use the threshold, we'll always use the bias.

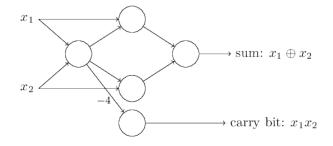
The NAND example shows that we can use perceptrons to compute simple logical functions. In fact, we can use networks of perceptrons to compute *any* logical function at all. The reason is that the NAND gate is universal for computation, that is, we can build any computation up out of NAND gates. For example, we can use NAND gates to build a circuit which adds two bits, x_1 and x_2 . This requires computing the bitwise sum, $x_1 \bigoplus x_2$, as well as a carry bit which is set to 1 when both x_1 and x_2 are 1, i.e., the carry bit is just the bitwise product x_1x_2 :



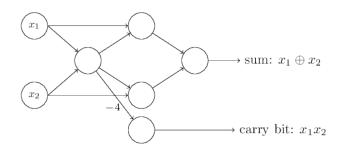
To get an equivalent network of perceptrons we replace all the NAND gates by perceptrons with two inputs, each with weight -2, and an overall bias of 3. Here's the resulting network. Note that I've moved the perceptron corresponding to the bottom right NAND gate a little, just to make it easier to draw the arrows on the diagram:



One notable aspect of this network of perceptrons is that the output from the leftmost perceptron is used twice as input to the bottommost perceptron. When I defined the perceptron model I didn't say whether this kind of double-output-to-the-same-place was allowed. Actually, it doesn't much matter. If we don't want to allow this kind of thing, then it's possible to simply merge the two lines, into a single connection with a weight of -4 instead of two connections with -2 weights. (If you don't find this obvious, you should stop and prove to yourself that this is equivalent.) With that change, the network looks as follows, with all unmarked weights equal to -2, all biases equal to 3, and a single weight of -4, as marked:



Up to now I've been drawing inputs like x_1 and x_2 as variables floating to the left of the network of perceptrons. In fact, it's conventional to draw an extra layer of perceptrons – the input layer – to encode the inputs:



This notation for input perceptrons, in which we have an output, but no inputs,



is a shorthand. It doesn't actually mean a perceptron with no inputs. To see this, suppose we did have a perceptron with no inputs. Then the weighted sum $\sum_j w_j x_j$ would always be zero, and so the perceptron would output 1 if b > 0, and 0 if $b \le 0$. That is, the perceptron would simply output a fixed value, not the desired value $(x_1, in the example$ above). It's better to think of the input perceptrons as not really being perceptrons at all, but rather special units which are simply defined to output the desired values, x_1, x_2, \ldots

The adder example demonstrates how a network of perceptrons can be used to simulate a circuit containing many NAND gates. And because NAND gates are universal for computation, it follows that perceptrons are also universal for computation.

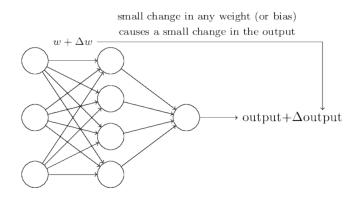
The computational universality of perceptrons is simultaneously reassuring and disappointing. It's reassuring because it tells us that networks of perceptrons can be as powerful as any other computing device. But it's also disappointing, because it makes it seem as though perceptrons are merely a new type of NAND gate. That's hardly big news!

However, the situation is better than this view suggests. It turns out that we can devise learning algorithms which can automatically tune the weights and biases of a network of artificial neurons. This tuning happens in response to external stimuli, without direct intervention by a programmer. These learning algorithms enable us to use artificial neurons in a way which is radically different to conventional logic gates. Instead of explicitly laying out a circuit of NAND and other gates, our neural networks can simply learn to solve problems, sometimes problems where it would be extremely difficult to directly design a conventional circuit.

3 Sigmoid neurons

Learning algorithms sound terrific. But how can we devise such algorithms for a neural network? 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!):

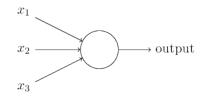


If it were true that a small change in a weight (or bias) causes only a small change in output, then we could use this fact to modify the weights and biases to get our network to behave more in the manner we want. For example, suppose the network was mistakenly classifying an image as an "8" when it should be a "9". We could figure out how to make a small change in the weights and biases so the network gets a little closer to classifying the image as a "9". And then we'd repeat this, changing the weights and biases over and over to produce better and better output. The network would be learning.

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. So while your "9" might now be classified correctly, the behaviour of the network on all the other images is likely to have completely changed in some hard-to-control way. That makes it difficult to see how to gradually modify the weights and biases so that the network gets closer to the desired behaviour. Perhaps there's some clever way of getting around this problem. But it's not immediately obvious how we can get a network of perceptrons to learn.

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 function¹, and is defined by:

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

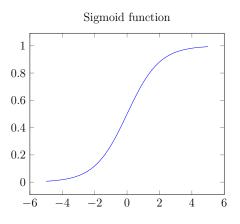
To put it all a little more explicitly, the output of a sigmoid neuron with inputs x_1, x_2, \ldots , weights w_1, w_2, \ldots , and bias b is

$$\frac{1}{1 + \exp\left(-\sum_{j} w_j x_j - b\right)}.$$
(4)

At first sight, sigmoid neurons appear very different to perceptrons. The algebraic form of the sigmoid function may seem opaque and forbidding if you're not already familiar with it. In fact, there are many similarities between perceptrons and sigmoid neurons, and the algebraic form of the sigmoid function turns out to be more of a technical detail than a true barrier to understanding.

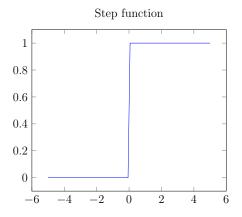
To understand the similarity to the perceptron model, suppose $z \equiv w \cdot x + b$ is a large positive number. Then $e^{-z} \approx 0$ and so $\sigma(z) \approx 1$. In other words, when $z = w \cdot x + b$ is large and positive, the output from the sigmoid neuron is approximately 1, just as it would 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 $\sigma(z) \approx 0$. So when $z = w \cdot x + b$ is very negative, the behaviour of a sigmoid neuron also closely approximates a perceptron. It's only when $w \cdot x + b$ is of modest size that there's much deviation from the perceptron model.

What about the algebraic form of σ ? How can we understand that? In fact, the exact form of σ isn't so important – what really matters is the shape of the function when plotted. Here's the shape:



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

¹Incidentally, σ is sometimes called the logistic function, and this new class of neurons called logistic neurons. It's useful to remember this terminology, since these terms are used by many people working with neural nets. However, we'll stick with the sigmoid terminology.



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 negative². By using the actual σ function we get, as already implied above, a smoothed out perceptron. Indeed, it's the smoothness of the σ function that is the crucial fact, not its detailed form. The smoothness of σ means that small changes Δw_j in the weights and Δb in the bias will produce a small change Δ output in the output from the neuron. In fact, calculus tells us that Δ output is well approximated by

$$\Delta \text{output} \approx \sum_{j} \frac{\partial \text{output}}{\partial w_j} \Delta w_j + \frac{\partial \text{output}}{\partial b} \Delta b \tag{5}$$

where the sum is over all the weights, w_j , and $\partial \operatorname{output}/\partial w_j$ and $\partial \operatorname{output}/\partial b$ denote partial derivatives of the output with respect to w_j and b, respectively. Don't panic if you're not comfortable with partial derivatives! While the expression above looks complicated, with all the partial derivatives, it's actually saying something very simple (and which is very good news): $\Delta \operatorname{output}$ is a linear function of the changes Δw_j and Δb in the weights and bias. This linearity makes it easy to choose small changes in the weights and biases to achieve any desired small change in the output. So while sigmoid neurons have much of the same qualitative behavior as perceptrons, they make 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 Equation (3)? In fact, later in the lecture notes we will occasionally consider neurons where the output is $f(w \cdot x + b)$ for some other activation function $f(\cdot)$. 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 later, using σ will simplify the algebra, simply because exponentials have lovely properties when differentiated. In any case, σ is commonly-used in work on neural nets, and is the activation function we'll use most often in this lecture notes.

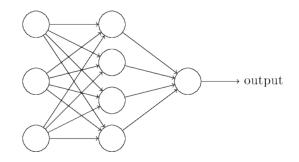
How should we interpret the output from a sigmoid neuron? Obviously, one big difference between perceptrons and sigmoid neurons is that sigmoid neurons don't just output 0 or 1. They can have as output any real number between 0 and 1, so values such as 0.173... and 0.689... are legitimate outputs. This can be useful, for example, if we want to use the output value to represent the average intensity of the pixels in an image input to a neural network. But sometimes it can be a nuisance. Suppose we want the

²Actually, when $w \cdot x + b = 0$ the perceptron outputs 0, while the step function outputs 1. So, strictly speaking, we'd need to modify the step function at that one point. But you get the idea.

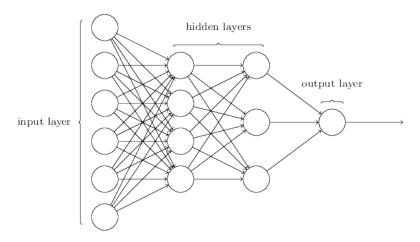
output from the network to indicate either "the input image is a 9" or "the input image is not a 9". Obviously, it'd be easiest to do this if the output was a 0 or a 1, as in a perceptron. But in practice we can set up a convention to deal with this, for example, by deciding to interpret any output of at least 0.5 as indicating a "9", and any output less than 0.5 as indicating "not a 9". I'll always explicitly state when we're using such a convention, so it shouldn't cause any confusion.

4 The architecture of neural networks

In the next section I'll introduce a neural network that can do a pretty good job classifying handwritten digits. In preparation for that, it helps to explain some terminology that lets us name different parts of a network. 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 term "hidden" perhaps sounds a little mysterious – the first time I heard the term I thought it must have some deep philosophical or mathematical significance – but it really means nothing more than "not an input or an output". The network above has just a single hidden layer, but some networks have multiple hidden layers. For example, the following four-layer network has two hidden 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. I'm not going to use the MLP terminology in this lecture notes, since I think it's confusing, but wanted to warn you of its existence. The design of the input and output layers in a network is often straightforward. For example, suppose we're trying to determine whether a handwritten image depicts a "9" or not. A natural way to design the network is to encode the intensities of the image pixels into the input neurons. If the image is a 64 by 64 greyscale image, then we'd have $4,096 = 64 \times 64$ input neurons, with the intensities scaled appropriately between 0 and 1. The output layer will contain just a single neuron, with output values of less than 0.5 indicating "input image is not a 9", and values greater than 0.5 indicating "input image is a 9".

While the design of the input and output layers of a neural network is often straightforward, there can be quite an art to the design of the hidden layers. In particular, it's not possible to sum up the design process for the hidden layers with a few simple rules of thumb. Instead, 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. We'll meet several such design heuristics later in this lecture notes.

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 – information is always fed forward, never fed back. If we did have loops, we'd end up with situations where the input to the σ function depended on the output. That'd be hard to make sense of, and so we don't allow such loops.

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.

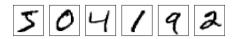
Recurrent neural nets have been less influential than feedforward networks, in part because the learning algorithms for recurrent nets are (at least to date) less powerful. But recurrent networks are still extremely interesting. They're much closer in spirit to how our brains work than feedforward networks.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

5 A simple network to classify handwritten digits

Having defined neural networks, let's return to handwriting recognition. 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. For example, we'd like to break the image

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into six separate images,



We humans solve this *segmentation problem* with ease, but it's challenging for a computer program to correctly break up the image. Once the image has been segmented, the program then needs to classify each individual digit. So, for instance, we'd like our program to recognize that the first digit above,

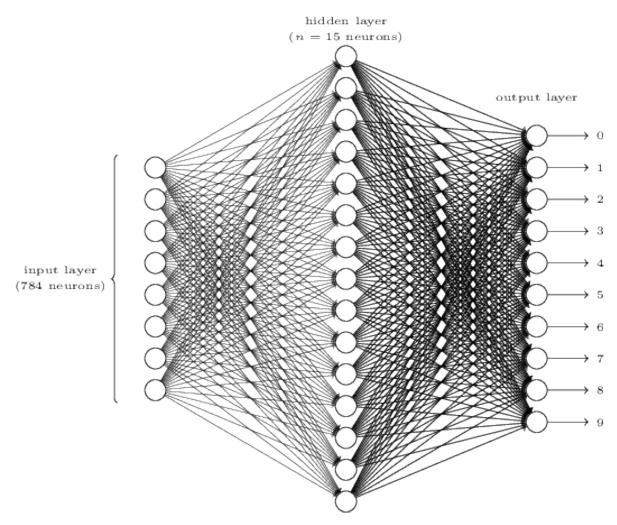
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is a 5.

We'll focus on writing a program to solve the second problem, that is, classifying individual digits. We do this because it turns out that the segmentation problem is not so difficult to solve, once you have a good way of classifying individual digits. There are many approaches to solving the segmentation problem. One approach is to trial many different ways of segmenting the image, using the individual digit classifier to score each trial segmentation. A trial segmentation gets a high score if the individual digit classifier is confident of its classification in all segments, and a low score if the classifier is having a lot of trouble in one or more segments. The idea is that if the classifier is having trouble somewhere, then it's probably having trouble because the segmentation has been chosen incorrectly. This idea and other variations can be used to solve the segmentation problem quite well. So instead of worrying about segmentation we'll concentrate on developing a neural network which can solve the more interesting and difficult problem, namely, recognizing individual handwritten digits.

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

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The input layer of the network contains neurons encoding the values of the input pixels. As discussed in the next section, our training data for the network will consist of many 28 by 28 pixel images of scanned handwritten digits, and so the input layer contains $784 = 28 \times 28$ neurons. For simplicity I've omitted most of the 784 input neurons in the diagram above. The input pixels are greyscale, 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. The example shown illustrates a small hidden layer, containing just n = 15 neurons.

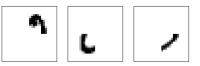
The output layer of the network contains 10 neurons. If the first neuron fires, i.e., has an output ≈ 1 , then that will indicate that the network thinks the digit is a 0. If the second neuron fires then that will indicate that the network thinks the digit is a 1. And so on. A little more precisely, we number the output neurons from 0 through 9, and figure out which neuron has the highest activation value. If that neuron is, say, neuron number 6, then our network will guess that the input digit was a 6. And so on for the other output neurons.

You might wonder why we use 10 output neurons. After all, the goal of the network is to tell us which digit (0, 1, 2, ..., 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 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 the 10 possible values for the input digit. Why should our network use 10 neurons instead? Isn't that inefficient? 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. Is there some heuristic that would tell us in advance that we should use the 10-output encoding instead of the 4-output encoding?

To understand why we do this, it helps to think about what the neural network is doing from first principles. Consider first the case where we use 10 output neurons. Let's concentrate on the first output neuron, the one that's trying to decide whether or not the digit is a 0. It does this by weighing up evidence from the hidden layer of neurons. What are those hidden neurons doing? Well, just suppose for the sake of argument that the first neuron in the hidden layer detects whether or not an image like the following is present:



It can do this by heavily weighting input pixels which overlap with the image, and only lightly weighting the other inputs. In a similar way, let's suppose for the sake of argument that the second, third, and fourth neurons in the hidden layer detect whether or not the following images are present:



As you may have guessed, these four images together make up the 0 image that we saw in the line of digits shown earlier:



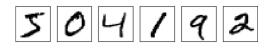
So if all four of these hidden neurons are firing then we can conclude that the digit is a 0. Of course, that's not the only sort of evidence we can use to conclude that the image was a 0 – we could legitimately get a 0 in many other ways (say, through translations of the above images, or slight distortions). But it seems safe to say that at least in this case we'd conclude that the input was a 0.

Supposing the neural network functions in this way, we can give a plausible explanation for why it's better to have 10 outputs from the network, rather than 4. 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. It's hard to imagine that there's any good historical reason the component shapes of the digit will be closely related to (say) the most significant bit in the output.

Now, with all that said, this is all just a heuristic. Nothing says that the three-layer neural network has to operate in the way I described, with the hidden neurons detecting simple component shapes. Maybe a clever learning algorithm will find some assignment of weights that lets us use only 4 output neurons. But as a heuristic the way of thinking I've described works pretty well, and can save you a lot of time in designing good neural network architectures.

6 Learning with gradient descent

Now that we have a design for our neural network, how can it learn to recognize digits? The first thing we'll need is a data set to learn from – a 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. MNIST's name comes from the fact that it is a modified subset of two data sets collected by NIST, the United States' National Institute of Standards and Technology. Here's a few images from MNIST:



As you can see, these digits are, in fact, the same as those shown at the beginning of this lecture notes as a challenge to recognize. Of course, when testing our network we'll ask it to recognize images which aren't in the training set!

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 greyscale 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 greyscale 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 grey 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 function³:

$$C(w,b) \equiv \frac{1}{2n} \sum_{x} \|y(x) - a\|^2$$
(6)

³Sometimes referred to as a loss or objective function. We use the term cost function throughout this lecture notes, but you should note the other terminology, since it's often used in research papers and other discussions of neural networks.

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, but to keep the notation simple I haven't explicitly indicated this dependence. 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 or just MSE. Inspecting the form of the quadratic cost function, we see that C(w, b) is non-negative, since every term in the sum is non-negative. Furthermore, the cost C(w, b) becomes small, i.e., $C(w, b) \approx 0$, 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. In other words, we want to find a set of weights and biases which make the cost as small as possible. We'll do that using an algorithm known as *qradient* descent.

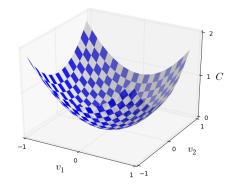
Why introduce the quadratic cost? After all, aren't we primarily interested in the number of images correctly classified by the network? Why not try to maximize that number directly, rather than minimizing a proxy measure like the quadratic cost? The problem with that is that the number of images correctly classified is not a smooth function of the weights and biases in the network. For the most part, making small changes to the weights and biases won't cause any change at all in the number of training images classified correctly. That makes it difficult to figure out how to change the weights and biases to get improved performance. If we instead use a smooth cost function like the quadratic cost it turns out to be easy to figure out how to make small changes in the weights and biases so as to get an improvement in the cost. That's why we focus first on minimizing the quadratic cost, and only after that will we examine the classification accuracy.

Even given that we want to use a smooth cost function, you may still wonder why we choose the quadratic function used in Equation (6). Isn't this a rather ad hoc choice? Perhaps if we chose a different cost function we'd get a totally different set of minimizing weights and biases? This is a valid concern, and later we'll revisit the cost function, and make some modifications. However, the quadratic cost function of Equation (6) works perfectly well for understanding the basics of learning in neural networks, so we'll stick with it for now.

Recapping, our goal in training a neural network is to find weights and biases which minimize the quadratic cost function C(w, b). This is a well-posed problem, but it's got a lot of distracting structure as currently posed – the interpretation of w and b as weights and biases, the σ function lurking in the background, the choice of network architecture, MNIST, and so on. It turns out that we can understand a tremendous amount by ignoring most of that structure, and just concentrating on the minimization aspect. So for now we're going to forget all about the specific form of the cost function, the connection to neural networks, and so on. Instead, we're going to imagine that we've simply been given a function of many variables and we want to minimize that function. We're going to develop a technique called gradient descent which can be used to solve such minimization problems. Then we'll come back to the specific function we want to minimize for neural networks.

Okay, let's suppose we're trying to minimize some function, C(v). This could be any

real-valued function of many variables, $v = v_1, v_2, \ldots$ Note that I've replaced the w and b notation by v to emphasize that this could be any function – we're not specifically thinking in the neural networks context any more. To minimize C(v) it helps to imagine C as a function of just two variables, which we'll call v_1 and v_2 :



What we'd like is to find where C achieves its global minimum. Now, of course, for the function plotted above, we can eyeball the graph and find the minimum. In that sense, I've perhaps shown slightly too simple a function! A general function, C, may be a complicated function of many variables, and it won't usually be possible to just eyeball the graph to find the minimum.

One way of attacking the problem is to use calculus to try to find the minimum analytically. We could compute derivatives and then try using them to find places where C is an extremum. 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!

(After asserting that we'll gain insight by imagining C as a function of just two variables, I've turned around twice in two paragraphs and said, "hey, but what if it's a function of many more than two variables?" Sorry about that. Please believe me when I say that it really does help to imagine C as a function of two variables. It just happens that sometimes that picture breaks down, and the last two paragraphs were dealing with such breakdowns. Good thinking about mathematics often involves juggling multiple intuitive pictures, learning when it's appropriate to use each picture, and when it's not.)

Okay, so calculus doesn't work. Fortunately, there is a beautiful analogy which suggests an algorithm which works pretty well. We start by thinking of our function as a kind of a valley. If you squint just a little at the plot above, that shouldn't be too hard. 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. Perhaps we can use this idea as a way to find a minimum for the function? We'd randomly choose a starting point for an (imaginary) ball, and then simulate the motion of the ball as it rolled down to the bottom of the valley. We could do this simulation simply by computing derivatives (and perhaps some second derivatives) of C – those derivatives would tell us everything we need to know about the local "shape" of the valley, and therefore how our ball should roll.

Based on what I've just written, you might suppose that we'll be trying to write down Newton's equations of motion for the ball, considering the effects of friction and gravity, and so on. Actually, we're not going to take the ball-rolling analogy quite that seriously – we're devising an algorithm to minimize C, not developing an accurate simulation of the laws of physics! The ball's-eye view is meant to stimulate our imagination, not constrain our thinking. So rather than get into all the messy details of physics, let's simply ask ourselves: if we were declared God for a day, and could make up our own laws of physics, dictating to the ball how it should roll, what law or laws of motion could we pick that would make it so the ball always rolled to the bottom of the valley?

To make this question more precise, 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:

$$\Delta C \approx \frac{\partial C}{\partial v_1} \Delta v_1 + \frac{\partial C}{\partial v_2} \Delta v_2. \tag{7}$$

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, $\Delta v \equiv (\Delta v_1, \Delta v_2)^T$, where T is again the transpose operation, turning row vectors into column vectors. We'll also define the gradient of C to be the vector of partial derivatives, $\left(\frac{\partial C}{\partial v_1}, \frac{\partial C}{\partial v_2}\right)^T$. We denote the gradient vector by ∇C , i.e.:

$$\nabla C \equiv \left(\frac{\partial C}{\partial v_1}, \frac{\partial C}{\partial v_2}\right)^T.$$
(8)

In a moment we'll rewrite the change ΔC in terms of Δv and the gradient, ∇C . Before getting to that, though, I want to clarify something that sometimes gets people hung up on the gradient. When meeting the ∇C notation for the first time, people sometimes wonder how they should think about the ∇ symbol. What, exactly, does ∇C mean? In fact, it's perfectly fine to think of ∇C as a single mathematical object – the vector defined above – which happens to be written using two symbols. In this point of view, ∇C is just a piece of notational flag-waving, telling you "hey, ∇C is a gradient vector". There are more advanced points of view where ∇C can be viewed as an independent mathematical entity in its own right (for example, as a differential operator), but we won't need such points of view.

With these definitions, the expression (7) for ΔC can be rewritten as

$$\Delta C \approx \nabla C \cdot \Delta v \tag{9}$$

This equation helps explain why ∇C is called the gradient vector: ∇C relates changes in v to changes in C, just as we'd expect something called a gradient to do. But what's really exciting about the equation is that it lets us see how to choose Δv so as to make ΔC negative. In particular, suppose we choose

$$\Delta v = -\eta \nabla C,\tag{10}$$

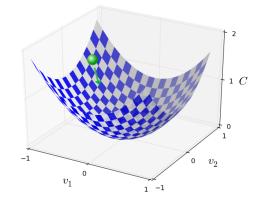
where η is a small, positive parameter (known as the *learning rate*). Then Equation (9) tells us that $\Delta C \approx -\eta \nabla C \cdot \nabla C = -\eta \|\nabla C\|^2$. Because $\|\nabla C\|^2 \ge 0$, this guarantees that $\Delta C \le 0$, i.e., C will always decrease, never increase, if we change v according to the

prescription in (10). (Within, of course, the limits of the approximation in Equation (9)). This is exactly the property we wanted! And so we'll take Equation (10) to define the "law of motion" for the ball in our gradient descent algorithm. That is, we'll use Equation (10) to compute a value for Δv , then move the ball's position v by that amount:

$$v \to v' = v - \eta \nabla C. \tag{11}$$

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. We can visualize it like this:



Notice that with this rule gradient descent doesn't reproduce real physical motion. In real life a ball has momentum, and that momentum may allow it to roll across the slope, or even (momentarily) roll uphill. It's only after the effects of friction set in that the ball is guaranteed to roll down into the valley. By contrast, our rule for choosing Δv just says "go down, right now". That's still a pretty good rule for finding the minimum!

To make gradient descent work correctly, we need to choose the learning rate η to be small enough that Equation (9) 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. In practical implementations, η is often varied so that Equation (9) remains a good approximation, but the algorithm isn't too slow. We'll see later how this works.

I've explained gradient descent when C is a function of just two variables. But, in fact, everything works just as well even when C is a function of many more variables. Suppose in particular that C is a function of m variables, v_1, \ldots, v_m . Then the change ΔC in C produced by a small change $\Delta v = (\Delta v_1, \ldots, \Delta v_m)^T$ is

$$\Delta C \approx \nabla C \cdot \Delta v, \tag{12}$$

where the gradient ∇C is the vector

$$\nabla C \equiv \left(\frac{\partial C}{\partial v_1}, \dots, \frac{\partial C}{\partial v_m}\right)^T.$$
(13)

Just as for the two variable case, we can choose

$$\Delta v = -\eta \nabla C,\tag{14}$$

and we're guaranteed that our (approximate) expression (12) for ΔC will be negative. This gives us a way of following the gradient to a minimum, even when C is a function of many variables, by repeatedly applying the update rule

$$v \to v' = v - \eta \nabla C. \tag{15}$$

You can think of this update rule as *defining* the gradient descent algorithm. It gives us a way of repeatedly changing the position v in order to find a minimum of the function C. The rule doesn't 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 lecture notes. 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.

Indeed, there's even a sense in which gradient descent is the optimal strategy for searching for a minimum. Let's suppose that we're trying to make a move Δv in position so as to decrease C as much as possible. This is equivalent to minimizing $\Delta C \approx \nabla C \cdot \Delta v$. We'll constrain the size of the move so that $\|\Delta v\| = \epsilon$ for some small fixed $\epsilon > 0$. In other words, we want a move that is a small step of a fixed size, and we're trying to find the movement direction which decreases C as much as possible. It can be proved that the choice of Δv which minimizes $\nabla C \cdot \Delta v$ is $\Delta v = -\eta \nabla C$, where $\eta = \epsilon/\|\nabla C\|$ is determined by the size constraint $\|\Delta v\| = \epsilon$. So gradient descent can be viewed as a way of taking small steps in the direction which does the most to immediately decrease C.

People have investigated many variations of gradient descent, including variations that more closely mimic a real physical ball. These ball-mimicking variations have some advantages, but also have a major disadvantage: it turns out to be necessary to compute second partial derivatives of C, and this can be quite costly. To see why it's costly, suppose we want to compute all the second partial derivatives $\partial^2 C/\partial v_j \partial v_k$. If there are a million such v_j variables then we'd need to compute something like a trillion (i.e., a million squared) second partial derivatives⁴! That's going to be computationally costly. With that said, there are tricks for avoiding this kind of problem, and finding alternatives to gradient descent is an active area of investigation. But in this lecture notes we'll use gradient descent (and variations) as our main approach to learning in neural networks.

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 (6). To see how this works, let's restate the gradient descent update rule, with the weights and biases replacing the variables v_j . In other words, our "position" now has components w_k and b_l , and the gradient vector ∇C has corresponding components $\partial C/\partial w_k$ and $\partial C/\partial b_l$. Writing out the gradient descent update rule in terms of components, we have

$$w_k \to w'_k = w_k - \eta \frac{\partial C}{\partial w_k}$$
 (16)

$$b_l \to b'_l = b_l - \eta \frac{\partial C}{\partial b_l}.$$
 (17)

⁴Actually, more like half a trillion, since $\partial^2 C / \partial v_i \partial v_k = \partial^2 C / \partial v_k \partial v_j$. Still, you get the point.

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.

There are a number of challenges in applying the gradient descent rule. We'll look into those in depth in later lecture notes. But for now I just want to mention one problem. To understand what the problem is, let's look back at the quadratic cost in Equation (6). 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. Provided the sample size m is large enough we expect that the average value of the ∇C_{X_j} will be roughly equal to the average over all ∇C_x , that is,

$$\frac{\sum_{j=1}^{m} \nabla C_{X_j}}{m} \approx \frac{\sum_x \nabla C_x}{n} = \nabla C,$$
(18)

where the second sum is over the entire set of training data. Swapping sides we get

$$\nabla C \approx \frac{1}{m} \sum_{j=1}^{m} \nabla C_{X_j},\tag{19}$$

confirming that we can estimate the overall gradient by computing gradients just for the randomly chosen mini-batch.

To connect this explicitly to learning in neural networks, suppose w_k and b_l denote the weights and biases in our neural network. Then stochastic gradient descent works by picking out a randomly chosen mini-batch of training inputs, and training with those,

$$w_k \to w'_k = w_k - \frac{\eta}{m} \sum_j \frac{\partial C_{X_j}}{\partial w_k}$$
 (20)

$$b_l \to b'_l = b_l - \frac{\eta}{m} \sum_j \frac{\partial C_{X_j}}{\partial b_l},$$
(21)

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.

Incidentally, it's worth noting that conventions vary about scaling of the cost function and of mini-batch updates to the weights and biases. In Equation (6) we scaled the overall cost function by a factor $\frac{1}{n}$. People sometimes omit the $\frac{1}{n}$, summing over the costs of individual training examples instead of averaging. This is particularly useful when the total number of training examples isn't known in advance. This can occur if more training data is being generated in real time, for instance. And, in a similar way, the mini-batch update rules (20) and (21) sometimes omit the $\frac{1}{m}$ term out the front of the sums. Conceptually this makes little difference, since it's equivalent to rescaling the learning rate η . But when doing detailed comparisons of different work it's worth watching out for.

We can think of stochastic gradient descent as being like political polling: it's much easier to sample a small mini-batch than it is to apply gradient descent to the full batch, just as carrying out a poll is easier than running a full election. 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, and it's the basis for most of the learning techniques we'll develop in this lecture notes.

Let me conclude this section by discussing a point that sometimes bugs people new to gradient descent. In neural networks the cost C is, of course, a function of many variables – all the weights and biases – and so in some sense defines a surface in a very high-dimensional space. Some people get hung up thinking: "Hey, I have to be able to visualize all these extra dimensions". And they may start to worry: "I can't think in four dimensions, let alone five (or five million)". Is there some special ability they're missing, some ability that "real" supermathematicians have? Of course, the answer is no. Even most professional mathematicians can't visualize four dimensions especially well, if at all. The trick they use, instead, is to develop other ways of representing what's going on. That's exactly what we did above: we used an algebraic (rather than visual) representation of ΔC to figure out how to move so as to decrease C. People who are good at thinking in high dimensions have a mental library containing many different techniques along these lines; our algebraic trick is just one example. Those techniques may not have the simplicity we're accustomed to when visualizing three dimensions, but once you build up a library of such techniques, you can get pretty good at thinking in high dimensions. I won't go into more detail here, but if you're interested then you may enjoy reading this discussion of some of the techniques professional mathematicians use to think in high dimensions. While some of the techniques discussed are quite complex. much of the best content is intuitive and accessible, and could be mastered by anyone.