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 apply it to a generic problem which is called classifying handwritten digits.

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 hand-writing recognizer by using thousands or even millions or billions of training examples.

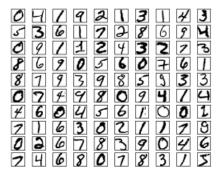


Figure 1: 100_handwritten_digits

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.

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:

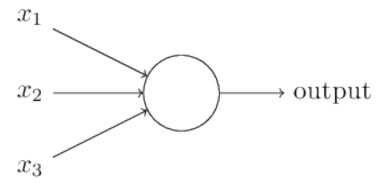


Figure 2: binary_inputs

In general it could have more or fewer inputs. Rosenblatt proposed a simple rule to compute the output. He introduced weights, w1,w2,..., 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 $\sum j \ wjx_j$ 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:

$$output = \begin{cases} 0, & if & \sum_{j} w_{j}x_{j} \leqslant threshold \\ 1, & if & \sum_{j} w_{j}x_{j} > threshold \end{cases}$$

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:

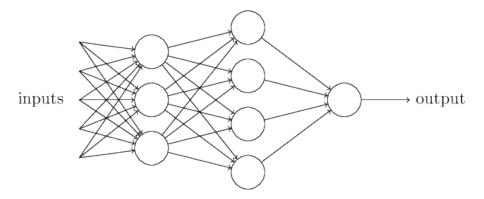


Figure 3: complex network

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 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 $\sum j \ wjx_j$ as a dot product, $w \cdot x \equiv \sum j \ wjx_j$, 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:

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

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.

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!):

small change in any weight (or bias)

causes a small change in the output $\longrightarrow \text{output} + \Delta \text{output}$

Figure 4: weight_small_change

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.

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:

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

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

$$\frac{1}{1 + \exp(\sum_{j} w_{j} x_{j} b)}$$

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:

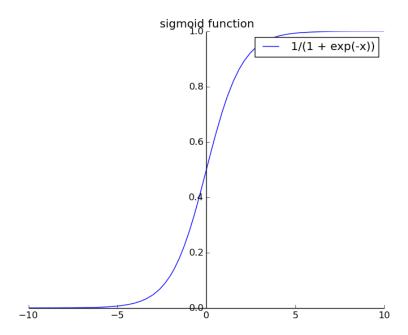
This shape is a smoothed out version of a step function or Heaviside step function:

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

$$\Delta output \approx \sum_{j} \frac{\partial \ output}{\partial w_{j}} \Delta w_{j} + \frac{\partial \ output}{\partial b} \Delta b$$

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



 $Figure \ 5: \ sigmoid_function$

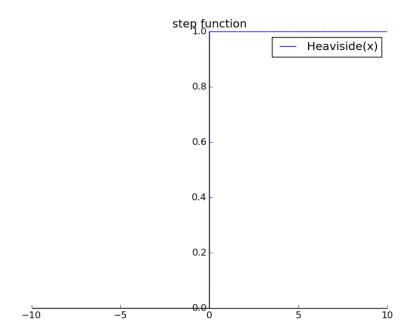


Figure 6: step_function

sigmoid neurons have much of the same qualitative behaviour 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 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.

$$\frac{d\sigma}{dz} = \left(1 - \frac{1}{1 + e^{-z}}\right) \left(\frac{1}{1 + e^{-z}}\right)$$
$$= (1 - \sigma)\sigma$$

The architecture of neural networks

Suppose we have the network:

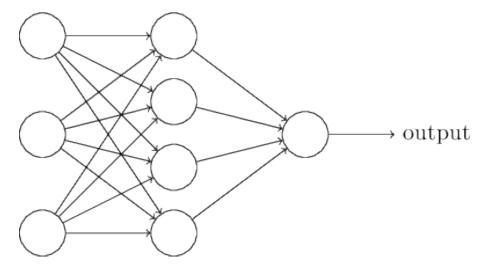


Figure 7: architecture

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

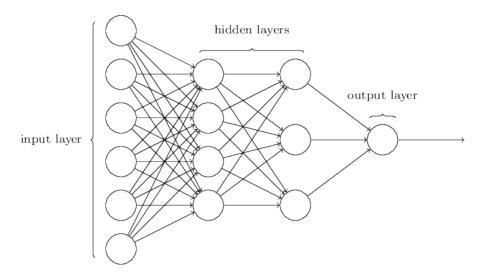


Figure 8: two hidden layers

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. It is not going to be used the MLP terminology in this book, 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.

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: digits sequence

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 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 24=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?

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

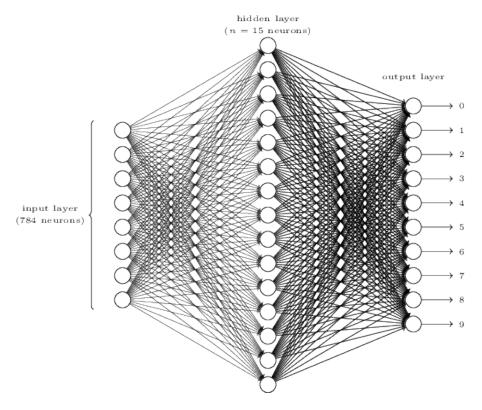


Figure 10: three_layer_neural_net

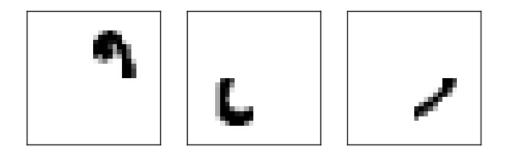


Figure 11: 0shapes

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.

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

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) = (0,0,0,0,0,1,0,0,0)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.

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

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 or just 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 = v1, v2, ...

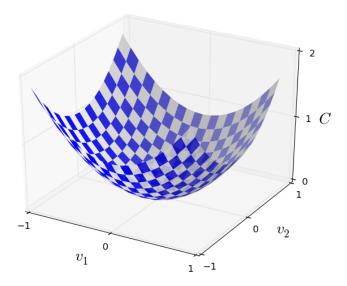


Figure 13: valley

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:

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

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.:

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

More generally, if C is function of m variables,

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

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

$$\Delta C \approx \nabla C \Delta v$$

In particular, suppose we choose,

$$\Delta v = \eta \nabla C$$

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

$$\Delta C \approx \eta \nabla C \cdot \nabla C = \eta ||\nabla C||^2$$

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:

$$v \to v' = v \eta \nabla C$$

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 (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.

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 .

$$w_k \to w_k' = w_k \eta \frac{\partial C}{\partial w_k} b_l \to b_l = b_l \eta \frac{\partial C}{\partial b_l}$$

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 $C=\frac{1}{n}\sum x\ Cx$, that is, it's an average over costs $C_x\frac{||y(x)a||^2}{2}$ 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, $\nabla C=\frac{1}{n}\sum x\ \nabla Cx$. 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.

$$\nabla C \approx \frac{1}{m} \sum_{i=1} \nabla C_{X_i}$$

Equation (17) depicts that overall gradient can be estimated just by randomly chosen mini-batch. And updating weights and biases is like below

$$w_k \to w_k' = w_k \frac{\eta}{m} \sum_j \frac{\partial C_{X_j}}{\partial w_k} b_l \to b_l = b_l \frac{\eta}{m} \sum_j \frac{\partial C_{X_j}}{\partial b_l}$$

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.

Implementing our network to classify digits

Get mnist loader.py and network.py from GitHub.

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.