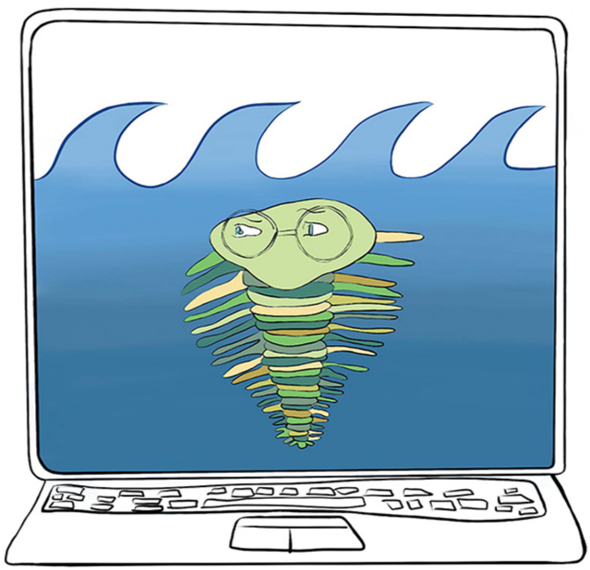
Addison Wesley Data & Analytics Series

DEEP LEARNING ILLUSTRATED

A Visual, Interactive Guide to Artificial Intelligence



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with GRANT BEYLEVELD *and* AGLAÉ BASSENS

FREE SAMPLE CHAPTER

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8

Training Deep Networks

In the preceding chapters, we described artificial neurons comprehensively and we walked through the process of forward propagating information through a network of neurons to output a prediction, such as whether a given fast food item is a hot dog, a juicy burger, or a greasy slice of pizza. In those culinary examples from Chapters 6 and 7, we fabricated numbers for the neuron parameters—the neuron weights and biases. In real-world applications, however, these parameters are not typically concocted arbitrarily: They are learned by training the network on data.

In this chapter, you will become acquainted with two techniques—called *gradient descent* and *backpropagation*—that work in tandem to learn artificial neural network parameters. As usual in this book, our presentation of these methods is not only theoretical: We provide pragmatic best practices for implementing the techniques. The chapter culminates in the application of these practices to the construction of a neural network with more than one hidden layer.

Cost Functions

In Chapter 7, you discovered that, upon forward propagating some input values all the way through an artificial neural network, the network provides its estimated output, which is denoted $\hat{y}$. If a network were perfectly calibrated, it would output $\hat{y}$ values that are exactly equal to the true label y. In our binary classifier for detecting hot dogs, for example (Figure 7.3), $y = 1$ indicated that the object presented to the network is a hot dog, while $y = 0$ indicated that it's something else. In an instance where we have in fact presented a hot dog to the network, therefore, ideally it would output $\hat{y} = 1$.

In practice, the gold standard of $\hat{y} = y$ is not always attained and so may be an excessively stringent definition of the "correct" $\hat{y}$. Instead, if $y = 1$ we might be quite pleased to see a $\hat{y}$ of, say, 0.9997, because that would indicate that the network has an extremely high confidence that the object is a hot dog. A $\hat{y}$ of 0.9 might be considered acceptable, $\hat{y} = 0.6$ to be disappointing, and $\hat{y} = 0.1192$ (as computed in Equation 7.7) to be awful.

To quantify the spectrum of output-evaluation sentiments from "quite pleased" all the way down to "awful," machine learning algorithms often involve *cost functions* (also known as *loss functions*). The two such functions that we cover in this book are called quadratic cost and cross-entropy cost. Let's cover them in turn.

Quadratic Cost

Quadratic cost is one of the simplest cost functions to calculate. It is alternatively called *mean squared error*, which handily describes all that there is to its calculation:

$$C = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \tag{8.1}$$

For any given instance i, we calculate the difference (the *error*) between the true label y_i and the network's estimated $\hat{y}_i$. We then *square* this difference, for two reasons:

1. Squaring ensures that whether y is greater than $\hat{y}$ or vice versa, the difference between the two is stated as a positive value.
2. Squaring penalizes large differences between y and $\hat{y}$ much more severely than small differences.

Having obtained a *squared error* for each instance i by using $(y_i - \hat{y}_i)^2$, we can then calculate the *mean* cost C across all n of our instances by:

1. Summing up cost across all instances using $\sum\limits_{i=1}^{n}$
2. Dividing by however many instances we have using $\frac{1}{n}$

By taking a peek inside the *Quadratic Cost* Jupyter notebook from the book's GitHub repo, you can play around with Equation 8.1 yourself. At the top of the notebook, we define a function to calculate the squared error for an instance i:

```
def squared_error(y, yhat):
    return (y - yhat)**2
```

By plugging a true `y` of `1` and the ideal `yhat` of `1` in to the function by using `squared_error(1, 1)`, we observe that—as desired—this perfect estimate is associated with a cost of `0`. Likewise, minor deviations from the ideal, such as a `yhat` of `0.9997`, correspond to an extremely small cost: `9.0e-08`.[1] As the difference between `y` and `yhat` increases, we witness the expected exponential increase in cost: Holding `y` steady at `1` but lowering `yhat` from `0.9` to `0.6`, and then to `0.1192`, the cost climbs increasingly rapidly from `0.01` to `0.16` and then to `0.78`. As a final bit of amusement in the notebook, we note that had `y` truly been `0`, our `yhat` of `0.1192` would be associated with a small cost: `0.0142`.

Saturated Neurons

While quadratic cost serves as a straightforward introduction to loss functions, it has a vital flaw. Consider Figure 8.1, in which we recapitulate the tanh activation function from Figure 6.10. The issue presented in the figure, called *neuron saturation*, is common across all activation functions, but we'll use tanh as our lone exemplar. A neuron is

1. `9.0e-08` is equivalent to 9.0×10^{-8}.

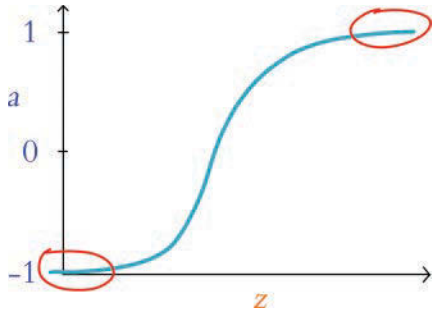

Figure 8.1 Plot reproducing the tanh activation function shown in Figure 6.10, drawing attention to the high and low values of z at which a neuron is saturated

considered saturated when the combination of its inputs and parameters (interacting as per "the most important equation," $z = w \cdot x + b$, which is captured in Figure 6.10) produces extreme values of z—the areas encircled with red in the plot in Figure 8.1. In these areas, changes in z (via adjustments to the neuron's underlying parameters w and b) cause only teensy-weensy changes in the neuron's activation a.[2]

Using methods that we cover later in this chapter—namely, gradient descent and backpropagation—a neural network is able to learn to approximate y through the tuning of the parameters w and b associated with all of its constituent neurons. In a saturated neuron, where changes to w and b lead to only minuscule changes in a, this learning slows to a crawl: If adjustments to w and b make no discernible impact on a given neuron's activation a, then these adjustments cannot have any discernible impact downstream (via forward propagation) on the network's $\hat{y}$, its estimate of y.

Cross-Entropy Cost

One of the ways[3] to minimize the impact of saturated neurons on learning speed is to use *cross-entropy cost* in lieu of quadratic cost. This alternative loss function is configured to enable efficient learning anywhere within the activation function curve of Figure 8.1. Because of this, it is a far more popular choice of cost function and it is the selection that predominates the remainder of this book.[4]

You need not preoccupy yourself with the equation for cross-entropy cost, but for the sake of completeness, here it is:

$$C = -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln \hat{y}_i + (1 - y_i)\ln(1 - \hat{y}_i)] \tag{8.2}$$

2. Recall from Chapter 6 that $a = \sigma(z)$, where σ is some activation function—in this example, the tanh function.
3. More methods for attenuating saturated neurons and their negative effects on a network are covered in Chapter 9.
4. Cross-entropy cost is well suited to neural networks solving classification problems, and such problems dominate this book. For regression problems (covered in Chapter 9), quadratic cost is a better option than cross-entropy cost.

The most pertinent aspects of the equation are:

- Like quadratic cost, divergence of $\hat{y}$ from y corresponds to increased cost.
- Analogous to the use of the square in quadratic cost, the use of the natural logarithm ln in cross-entropy cost causes larger differences between $\hat{y}$ and y to be associated with exponentially larger cost.
- Cross-entropy cost is structured so that the larger the difference between $\hat{y}$ and y, *the faster the neuron is able to learn*.[5]

To make it easier to remember that the greater the cost, the more quickly a neural network incorporating cross-entropy cost learns, here's an analogy that would absolutely never involve any of your esteemed authors: Let's say you're at a cocktail party leading the conversation of a group of people that you've met that evening. The strong martini you're holding has already gone to your head, and you go out on a limb by throwing a risqué line into your otherwise charming repartee. Your audience reacts with immediate, visible disgust. With this response clearly indicating that your quip was well off the mark, you learn pretty darn quickly. It's exceedingly unlikely you'll be repeating the joke anytime soon.

Anyway, that's plenty enough on disasters of social etiquette. The final item to note on cross-entropy cost is that, by including $\hat{y}$, the formula provided in Equation 8.2 applies to only the output layer. Recall from Chapter 7 (specifically the discussion of Figure 7.3) that $\hat{y}$ is a special case of a: It's actually just another plain old a value—except that it's being calculated by neurons in the output layer of a neural network. With this in mind, Equation 8.2 could be expressed with a_i substituted in for $\hat{y}_i$ so that the equation generalizes neatly beyond the output layer to neurons in any layer of a network:

$$C = -\frac{1}{n}\sum_{i=1}^{n}[y_i \ln a_i + (1 - y_i)\ln(1 - a_i)] \tag{8.3}$$

To cement all of this theoretical chatter about cross-entropy cost, let's interactively explore our aptly named *Cross Entropy Cost* Jupyter notebook. There is only one dependency in the notebook: the `log` function from the *NumPy* package, which enables us to compute the natural logarithm ln shown twice in Equation 8.3. We load this dependency using `from numpy import log`.

Next, we define a function for calculating cross-entropy cost for an instance i:

```
def cross_entropy(y, a):
    return -1*(y*log(a) + (1-y)*log(1-a))
```

5. To understand how the cross-entropy cost function in Equation 8.2 enables a neuron with larger cost to learn more rapidly, we require a touch of partial-derivative calculus. (Because we endeavor to minimize the use of advanced mathematics in this book, we've relegated this calculus-focused explanation to this footnote.) Central to the two computational methods that enable neural networks to learn—gradient descent and backpropagation—is the comparison of the rate of change of cost C relative to neuron parameters like weight w. Using partial-derivative notation, we can represent these relative rates of change as $\frac{\partial C}{\partial w}$. The cross-entropy cost function is deliberately structured so that, when we calculate its derivative, $\frac{\partial C}{\partial w}$ is related to $(\hat{y} - y)$. Thus, the larger the difference between the ideal output y and the neuron's estimated output $\hat{y}$, the greater the rate of change of cost C with respect to weight w.

Table 8.1 Cross-entropy costs associated with selected example inputs

y	a	C
1	0.9997	0.0003
1	0.9	0.1
1	0.6	0.5
1	0.1192	2.1
0	0.1192	0.1269
1	1−0.1192	0.1269

Plugging the same values in to our `cross_entropy()` function as we did the `squared_error()` function earlier in this chapter, we observe comparable behavior. As shown in Table 8.1, by holding y steady at `1` and gradually decreasing a from the nearly ideal estimate of `0.9997` downward, we get exponential increases in cross-entropy cost. The table further illustrates that—again, consistent with the behavior of its quadratic cousin—cross-entropy cost would be low, with an a of `0.1192`, if y happened to in fact be `0`. These results reiterate for us that the chief distinction between the quadratic and cross-entropy functions is not the particular cost value that they calculate per se, but rather it is the rate at which they learn within a neural net—especially if saturated neurons are involved.

Optimization: Learning to Minimize Cost

Cost functions provide us with a quantification of how incorrect our model's estimate of the ideal y is. This is most helpful because it arms us with a metric we can leverage to reduce our network's incorrectness.

As alluded to a couple of times in this chapter, the primary approach for minimizing cost in deep learning paradigms is to pair an approach called gradient descent with another one called backpropagation. These approaches are *optimizers* and they enable the network to *learn*. This learning is accomplished by adjusting the model's parameters so that its estimated $\hat{y}$ gradually converges toward the target of y, and thus the cost decreases. We cover gradient descent first and move on to backpropagation immediately afterward.

Gradient Descent

Gradient descent is a handy, efficient tool for adjusting a model's parameters with the aim of minimizing cost, particularly if you have a lot of training data available. It is widely used across the field of machine learning, not only in deep learning.

In Figure 8.2, we use a nimble trilobite in a cartoon to illustrate how gradient descent works. Along the horizontal axis in each frame is some parameter that we've denoted as p. In an artificial neural network, this parameter would be either a neuron's weight w or bias b. In the top frame, the trilobite finds itself on a hill. Its goal is to *descend* the gradient, thereby finding the location with the minimum cost, C. But there's a twist: The trilobite

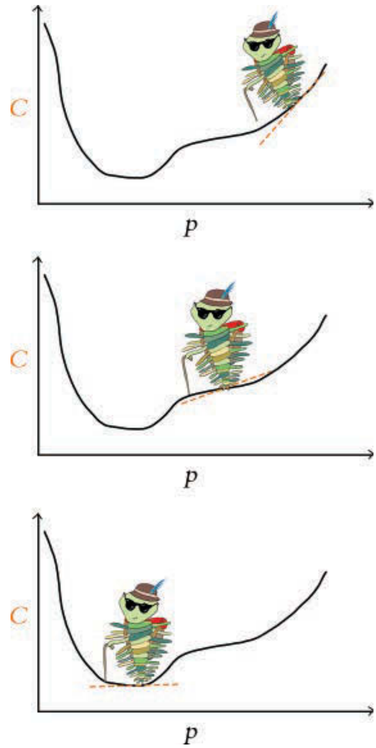

Figure 8.2 A trilobite using gradient descent to find the value of a parameter p associated with minimal cost, C

is blind! It cannot see whether deeper valleys lie far away somewhere, and so it can only use its cane to investigate the slope of the terrain in its immediate vicinity.

The dashed orange line in Figure 8.2 indicates the blind trilobite's calculation of the slope at the point where it finds itself. According to that slope line, if the trilobite takes a step to the left (i.e., to a slightly lower value of p), it would be moving to a location with smaller cost. On the hand, if the trilobite takes a step to the right (a slightly *higher* value of p), it would be moving to a location with *higher* cost. Given the trilobite's desire to descend the gradient, it chooses to take a step to the left.

By the middle frame, the trilobite has taken several steps to the left. Here again, we see it evaluating the slope with the orange line and discovering that, yet again, a step to the left will bring it to a location with lower cost, and so it takes another step left. In the lower frame, the trilobite has succeeded in making its way to the location—the value of the parameter p—corresponding to the minimum cost. From this position, if it were to take a step to the left *or* to the right, cost would go up, so it gleefully remains in place.

In practice, a deep learning model would not have only one parameter. It is not uncommon for deep learning networks to have millions of parameters, and some industrial applications have billions of them. Even our *Shallow Net in Keras*—one of the smallest models we build in this book—has 50,890 parameters (see Figure 7.5).

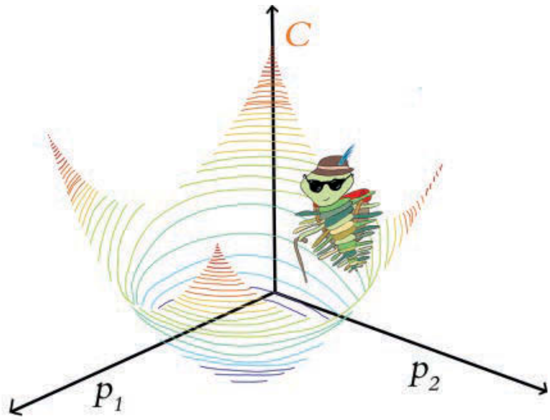

Figure 8.3 A trilobite exploring along two model parameters—p_1 and p_2—in order to minimize cost via gradient descent. In a mountain-adventure analogy, p_1 and p_2 could be thought of as latitude and longitude, and altitude represents cost.

Although it's impossible for the human mind to imagine a billion-dimensional space, the two-parameter cartoon shown in Figure 8.3 provides a sense of how gradient descent scales up to minimize cost across multiple parameters simultaneously. Across however many trainable parameters there are in a model, gradient descent iteratively evaluates slopes[6] to identify the adjustments to those parameters that correspond to the steepest reduction in cost. With two parameters, as in the trilobite cartoon in Figure 8.3, for example, this procedure can be likened to a blind hike through the mountains, where:

- Latitude represents one parameter, say p_1.
- Longitude represents the other parameter, p_2.
- Altitude represents cost—the lower the altitude, the better!

The trilobite randomly finds itself at a location in the mountains. From that point, it feels around with its cane to identify the direction of the step it can take that will reduce its altitude the most. It then takes that single step. Repeating this process many times, the trilobite may eventually find itself at the latitude and longitude coordinates that correspond to the lowest-possible altitude (the minimum cost), at which point the trilobite's surreal alpine adventure is complete.

Learning Rate

For conceptual simplicity, in Figure 8.4, let's return to a blind trilobite navigating a single-parameter world instead of a two-parameter world. Now let's imagine that we have a ray-gun that can shrink or enlarge trilobites. In the middle panel, we've used our ray-gun to make our trilobite very small. The trilobite's steps will then be correspondingly small, and so it will take our intrepid little hiker a long time to find its way to the

6. Using partial-derivative calculus.

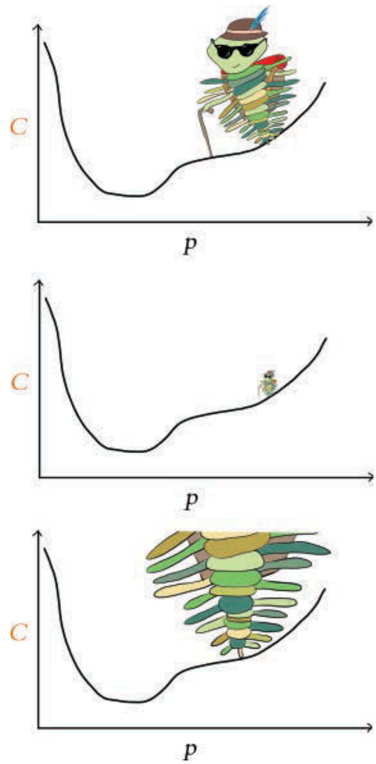

Figure 8.4 The learning rate (η) of gradient descent expressed as the size of a trilobite. The middle panel has a small learning rate, and the bottom panel, a large one.

legendary valley of minimum cost. On the other hand, consider the bottom panel, in which we've used our ray-gun to make the trilobite very large. The situation here is even worse! The trilobite's steps will now be so large that it will step right over the valley of minimum cost, and so it never has any hope of finding it.

In gradient descent terminology, step size is referred to as *learning rate* and denoted with the Greek letter η (eta, pronounced "ee-ta"). Learning rate is the first of several model *hyperparameters* that we cover in this book. In machine learning, including deep learning, hyperparameters are aspects of the model that we configure before we begin training the model. So hyperparameters such as η are preset while, in contrast, parameters—namely, w and b—are learned during training.

Getting your hyperparameters right for a given deep learning model often requires some trial and error. For the learning rate η, it's something like the fairy tale of "Goldilocks and the Three Bears": Too small and too large are both inadequate, but there's a sweet spot in the middle. More specifically, as we portray in Figure 8.4, if η is too small, then it will take many, many iterations of gradient descent (read: an unnecessarily long time) to reach the minimal cost. On the other hand, selecting a value for η

that is too large means we might never reach minimal cost at all: The gradient descent algorithm will act erratically as it jumps right over the parameters associated with minimal cost.

Coming up in Chapter 9, we have a clever trick waiting for you that will circumnavigate the need for you to manually select a given neural network's η hyperparameter. In the interim, however, here are our rules of thumb on the topic:

- Begin with a learning rate of about 0.01 or 0.001.
- If your model is able to learn (i.e., if cost decreases consistently epoch over epoch) but training happens very slowly (i.e., each epoch, the cost decreases only a small amount), then increase your learning rate by an order of magnitude (e.g., from 0.01 to 0.1). If the cost begins to jump up and down erratically epoch over epoch, then you've gone too far, so rein in your learning rate.
- At the other extreme, if your model is unable to learn, then your learning rate may be too high. Try decreasing it by orders of magnitude (e.g., from 0.001 to 0.0001) until cost decreases consistently epoch over epoch. For a visual, interactive way to get a handle on the erratic behavior of a model when its learning rate is too high, you can return to the TensorFlow Playground example from Figure 1.18 and dial up the value within the "Learning rate" dropdown box.

Batch Size and Stochastic Gradient Descent

When we introduced gradient descent, we suggested that it is efficient for machine learning problems that involve a large dataset. In the strictest sense, we outright lied to you. The truth is that if we have a very large quantity of training data, *ordinary* gradient descent would not work at all because it wouldn't be possible to fit all of the data into the memory (RAM) of our machine.

Memory isn't the only potential snag; compute power could cause us headaches, too. A relatively large dataset might squeeze into the memory of our machine, but if we tried to train a neural network containing millions of parameters with all those data, vanilla gradient descent would be highly *in*efficient because of the computational complexity of the associated high-volume, high-dimensional calculations.

Thankfully, there's a solution to these memory and compute limitations: the *stochastic* variant of gradient descent. With this variation, we split our training data into *mini-batches*—small subsets of our full training dataset—to render gradient descent both manageable and productive.

Although we didn't focus on it at the time, when we trained the model in our *Shallow Net in Keras* notebook back in Chapter 5 we were already using stochastic gradient descent by setting our `optimizer` to `SGD` in the `model.compile()` step. Further, in the subsequent line of code when we called the `model.fit()` method, we set `batch_size` to `128` to specify the size of our mini-batches—the number of training data points that we use for a given iteration of SGD. Like the learning rate η presented earlier in this chapter, *batch size* is also a model hyperparameter.

Let's work through some numbers to make the concepts of batches and stochastic gradient descent more tangible. In the MNIST dataset, there are 60,000 training images.

With a batch size of 128 images, we then have $\lceil 468.75 \rceil = 469$ batches[7,8] of gradient descent per epoch:

$$\begin{aligned} \text{number of batches} &= \left\lceil \frac{\text{size of training dataset}}{\text{batch size}} \right\rceil \\ &= \left\lceil \frac{60,000 \text{ images}}{128 \text{ images}} \right\rceil \\ &= \lceil 468.75 \rceil \\ &= 469 \end{aligned} \tag{8.4}$$

Before carrying out any training, we initialize our network with random values for each neuron's parameters w and b.[9] To begin the first epoch of training:

1. We shuffle and divide the training images into mini-batches of 128 images each. These 128 MNIST images provide 784 pixels each, which all together constitute the inputs x that are passed into our neural network. It's this shuffling step that puts the *stochastic* (which means *random*) in "stochastic gradient descent."
2. By forward propagation, information about the 128 images is processed by the network, layer through layer, until the output layer ultimately produces $\hat{y}$ values.
3. A cost function (e.g., cross-entropy cost) evaluates the network's $\hat{y}$ values against the true y values, providing a cost C for this particular mini-batch of 128 images.
4. To minimize cost and thereby improve the network's estimates of y given x, the gradient descent part of stochastic gradient descent is performed: Every single w and b parameter in the network is adjusted proportional to how much each contributed to the error (i.e., the cost) in this batch (note that the adjustments are scaled by the learning rate hyperparameter η).[10]

These four steps constitute a *round of training*, as summarized by Figure 8.5.

Figure 8.6 captures how rounds of training are repeated until we run out of training images to sample. The sampling in step 1 is done *without replacement*, meaning that at the end of an epoch each image has been seen by the algorithm only once, and yet between different epochs the mini-batches are sampled randomly. After a total of 468 rounds, the final batch contains only 96 samples.

This marks the end of the first epoch of training. Assuming we've set our model up to train for further epochs, we begin the next epoch by replenishing our pool with all 60,000 training images. As we did through the previous epoch, we then proceed through a further 469 rounds of stochastic gradient descent.[11] Training continues in this way until the total desired number of epochs is reached.

7. Because 60,000 is not perfectly divisible by 128, that 469th batch would contain only $0.75 \times 128 = 96$ images.
8. The square brackets we use here and in Equation 8.4 that appear to be missing the horizontal element from the bottom are used to denote the calculation of an integer-value ceiling. The whole-integer ceiling of 468.75, for example, is 469.
9. We delve into the particulars of parameter initialization with random values in Chapter 9.
10. This error-proportional adjustment is calculated during backpropagation. We haven't covered backpropagation explicitly yet, but it's coming up in the next section, so hang on tight!
11. Because we're sampling randomly, the order in which we select training images for our 469 mini-batches is completely different for every epoch.

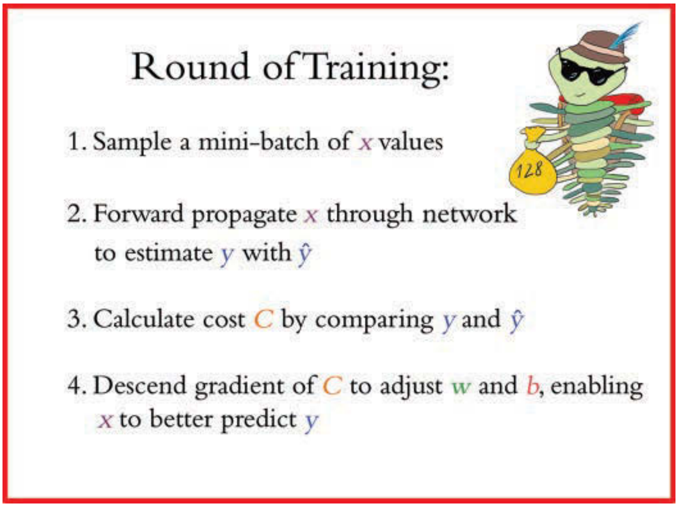

Figure 8.5 An individual round of training with stochastic gradient descent. Although mini-batch size is a hyperparameter that can vary, in this particular case, the mini-batch consists of 128 MNIST digits, as exemplified by our hike-loving trilobite carrying a small bag of data.

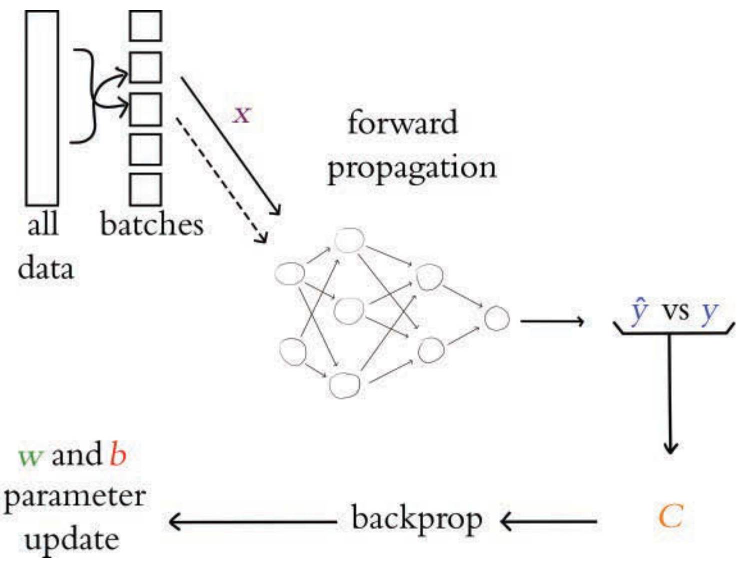

Figure 8.6 An outline of the overall process for training a neural network with stochastic gradient descent. The entire dataset is shuffled and split into batches. Each batch is forward propagated through the network; the output $\hat{y}$ is compared to the ground truth y and the cost C is calculated; backpropagation calculates the gradients; and the model parameters w and b are updated. The next batch (indicated by a dashed line) is forward propagated, and so on until all of the batches have moved through the network. Once all the batches have been used, a single epoch is complete and the process starts again with a reshuffling of the full training dataset.

The total *number of epochs* that we set our network to train for is yet another hyperparameter, by the way. This hyperparameter, though, is one of the easiest to get right:

- If the cost on your validation data is going down epoch over epoch, and if your final epoch attained the lowest cost yet, then you can try training for additional epochs.
- Once the cost on your validation data begins to creep upward, that's an indicator that your model has begun to *overfit* to your training data because you've trained for too many epochs. (We elaborate much more on overfitting in Chapter 9.)
- There are methods[12] you can use to automatically monitor training and validation cost and stop training early if things start to go awry. In this way, you could set the number of epochs to be arbitrarily large and know that training will continue until the validation cost stops improving—and certainly before the model begins overfitting!

Escaping the Local Minimum

In all of the examples of gradient descent thus far in the chapter, our hiking trilobite has encountered no hurdles on its journey toward minimum cost. There are no guarantees that this would be the case, however. Indeed, such smooth sailing is unusual.

Figure 8.7 shows the mountaineering trilobite exploring the cost of some new model that is being used to solve some new problem. With this new problem, the relationship between the parameter p and cost C is more complex. To have our neural network estimate y as accurately as possible, gradient descent needs to identify the parameter values associated with the lowest-attainable cost. However, as our trilobite makes its way from its random starting point in the top panel, gradient descent leads it to getting trapped in a *local minimum*. As shown in the middle panel, while our intrepid explorer is in the local minimum, a step to the left or a step to the right both lead to an increase in cost, and so the blind trilobite stays put, completely oblivious of the existence of a deeper valley—the *global minimum*—lying yonder.

All is not lost, friends, for stochastic gradient descent comes to the rescue here again. The sampling of mini-batches can have the effect of smoothing out the cost curve, as exemplified by the dashed curve shown in the bottom panel of Figure 8.7. This smoothing happens because the estimate is noisier when estimating the gradient from a smaller mini-batch (versus from the entire dataset). Although the actual gradient in the local minimum truly is zero, estimates of the gradient from small subsets of the data don't provide the complete picture and might give an inaccurate reading, causing our trilobite to take a step left thinking there is a gradient when there really isn't one. This noisiness and inaccuracy is paradoxically a good thing! The incorrect gradient may result in a step that is large enough for the trilobite to escape the local valley and continue making its way down the mountain. Thus, by estimating the gradient many times on these mini-batches, the noise is smoothed out and we are able to avoid local minima. In summary, although each mini-batch on its own lacks complete information about the cost curve, in the long run—over a large number of mini-batches—this tends to work to our advantage.

12. See `keras.io/callbacks/#earlystopping`.

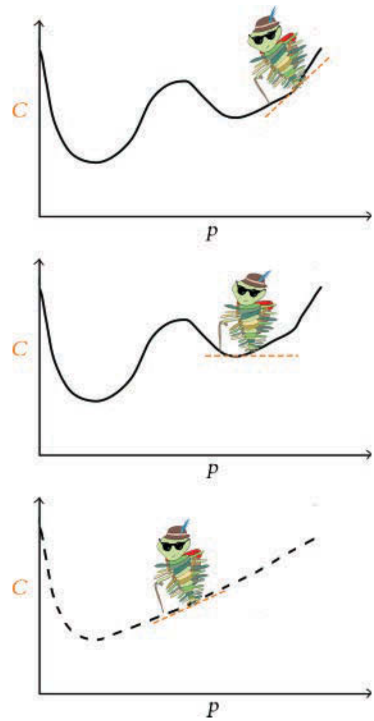

Figure 8.7 A trilobite applying vanilla gradient descent from a random starting point (top panel) is ensnared by a local minimum of cost (middle panel). By turning to stochastic gradient descent in the bottom panel, the daring trilobite is able to bypass the local minimum and make its way toward the global minimum.

Like the learning rate hyperparameter η, there is also a Goldilocks-style sweet spot for batch size. If the batch size is too large, the estimate of the gradient of the cost function is far more accurate. In this way, the trilobite has a more exacting impression of the gradient in its immediate vicinity and is able to take a step (proportional to η) in the direction of the steepest possible descent. However, the model is at risk of becoming trapped in local minima as described in the preceding paragraph.[13] Besides that, the model might not fit in memory on your machine, and the compute time per iteration of gradient descent could be very long.

On the other hand, if the batch size is too small, each gradient estimate may be excessively noisy (because a very small subset of the data is being used to estimate the gradient of the entire dataset) and the corresponding path down the mountain will be unnecessarily circuitous; training will take longer because of these erratic gradient descent steps. Furthermore, you're not taking advantage of the memory and compute resources on your

13. It's worth noting that the learning rate η plays a role here. If the size of the local minimum was *smaller* than the step size, the trilobite would likely breeze right past the local minimum, akin to how we step over cracks in the sidewalk.

machine.[14] With that in mind, here are our rules of thumb for finding the batch-size sweet spot:

- Start with a batch size of 32.
- If the mini-batch is too large to fit into memory on your machine, try decreasing your batch size by powers of 2 (e.g., from 32 to 16).
- If your model trains well (i.e., cost is going down consistently) but each epoch is taking very long and you are aware that you have RAM to spare,[15] you could experiment with increasing your batch size. To avoid getting trapped in local minima, we don't recommend going beyond 128.

Backpropagation

Although stochastic gradient descent operates well on its own to adjust parameters and minimize cost in many types of machine learning models, for deep learning models in particular there is an extra hurdle: We need to be able to efficiently adjust parameters *through multiple layers* of artificial neurons. To do this, stochastic gradient descent is partnered up with a technique called *backpropagation*.

Backpropagation—or backprop for short—is an elegant application of the "chain rule" from calculus.[16] As shown along the bottom of Figure 8.6 and as suggested by its very name, backpropagation courses through a neural network in the opposite direction of forward propagation. Whereas forward propagation carries information about the input $\boldsymbol{x}$ through successive layers of neurons to approximate $\boldsymbol{y}$ with $\hat{\boldsymbol{y}}$, backpropagation carries information about the cost $\boldsymbol{C}$ *backwards* through the layers in reverse order and, with the overarching aim of reducing cost, adjusts neuron parameters throughout the network.

Although the nitty-gritty of backpropagation has been relegated to Appendix B, it's worth understanding (in broad strokes) what the backpropagation algorithm does: Any given neural network model is randomly initialized with parameter ($\boldsymbol{w}$ and $\boldsymbol{b}$) values (such initialization is detailed in Chapter 9). Thus, prior to any training, when the first $\boldsymbol{x}$ value is fed in, the network outputs a random guess at $\hat{\boldsymbol{y}}$. This is unlikely to be a good guess, and the cost associated with this random guess will probably be high. At this point, we need to update the weights in order to minimize the cost—the very essence of machine learning. To do this within a neural network, we use backpropagation to calculate the *gradient* of the cost function with respect to each weight in the network.

14. Stochastic gradient descent with a batch size of 1 is known as *online learning*. It's worth noting that this is not the fastest method in terms of compute. The matrix multiplication associated with each round of mini-batch training is highly optimized, and so training can be several orders of magnitude quicker when using moderately sized mini-batches relative to online learning.

15. On a Unix-based operating system, including macOS, RAM usage may be assessed by running the `top` or `htop` command within a Terminal window.

16. To elucidate the mathematics underlying backpropagation, a fair bit of partial-derivative calculus is necessary. While we encourage the development of an in-depth understanding of the beauty of backprop, we also appreciate that calculus might not be the most appetizing topic for everyone. Thus, we've placed our content on backprop mathematics in Appendix B.