5 Multilayer Perceptrons

In this chapter, we will introduce your first truly *deep* network. The simplest deep networks are called *multilayer perceptrons*, and they consist of multiple layers of neurons each fully connected to those in the layer below (from which they receive input) and those above (which they, in turn, influence). Although automatic differentiation significantly simplifies the implementation of deep learning algorithms, we will dive deep into how these gradients are calculated in deep networks. Then we will be ready to discuss issues relating to numerical stability and parameter initialization that are key to successfully training deep networks. When we train such high-capacity models we run the risk of overfitting. Thus, we will revisit regularization and generalization for deep networks. Throughout, we aim to give you a firm grasp not just of the concepts but also of the practice of using deep networks. At the end of this chapter, we apply what we have introduced so far to a real case: house price prediction. We punt matters relating to the computational performance, scalability, and efficiency of our models to subsequent chapters.

5.1 Multilayer Perceptrons

In Section 4.1, we introduced softmax regression, implementing the algorithm from scratch (Section 4.4) and using high-level APIs (Section 4.5). This allowed us to train classifiers capable of recognizing 10 categories of clothing from low-resolution images. Along the way, we learned how to wrangle data, coerce our outputs into a valid probability distribution, apply an appropriate loss function, and minimize it with respect to our model's parameters. Now that we have mastered these mechanics in the context of simple linear models, we can launch our exploration of deep neural networks, the comparatively rich class of models with which this book is primarily concerned.

```
%matplotlib inline
import torch
from d2l import torch as d2l
```

5.1.1 Hidden Layers

We described affine transformations in Section 3.1.1 as linear transformations with added bias. To begin, recall the model architecture corresponding to our softmax regression example, illustrated in Fig. 4.1.1. This model maps inputs directly to outputs via a single affine transformation, followed by a softmax operation. If our labels truly were related to the input data by a simple affine transformation, then this approach would be sufficient. However, linearity (in affine transformations) is a *strong* assumption.

Limitations of Linear Models

For example, linearity implies the *weaker* assumption of *monotonicity*, i.e., that any increase in our feature must either always cause an increase in our model's output (if the corresponding weight is positive), or always cause a decrease in our model's output (if the corresponding weight is negative). Sometimes that makes sense. For example, if we were trying to predict whether an individual will repay a loan, we might reasonably assume that all other things being equal, an applicant with a higher income would always be more likely to repay than one with a lower income. While monotonic, this relationship likely is not linearly associated with the probability of repayment. An increase in income from \$0 to \$50,000 likely corresponds to a bigger increase in likelihood of repayment than an increase from \$1 million to \$1.05 million. One way to handle this might be to postprocess our outcome such that linearity becomes more plausible, by using the logistic map (and thus the logarithm of the probability of outcome).

Note that we can easily come up with examples that violate monotonicity. Say for example that we want to predict health as a function of body temperature. For individuals with a normal body temperature above 37°C (98.6°F), higher temperatures indicate greater risk. However, if the body temperatures drops below 37°C, lower temperatures indicate greater risk! Again, we might resolve the problem with some clever preprocessing, such as using the distance from 37°C as a feature.

But what about classifying images of cats and dogs? Should increasing the intensity of the pixel at location (13, 17) always increase (or always decrease) the likelihood that the image depicts a dog? Reliance on a linear model corresponds to the implicit assumption that the only requirement for differentiating cats and dogs is to assess the brightness of individual pixels. This approach is doomed to fail in a world where inverting an image preserves the category.

And yet despite the apparent absurdity of linearity here, as compared with our previous examples, it is less obvious that we could address the problem with a simple preprocessing fix. That is, because the significance of any pixel depends in complex ways on its context (the values of the surrounding pixels). While there might exist a representation of our data that would take into account the relevant interactions among our features, on top of which a linear model would be suitable, we simply do not know how to calculate it by hand. With deep neural networks, we used observational data to jointly learn both a representation via hidden layers and a linear predictor that acts upon that representation.

This problem of nonlinearity has been studied for at least a century (Fisher, 1925). For instance, decision trees in their most basic form use a sequence of binary decisions to decide upon class membership (Quinlan, 1993). Likewise, kernel methods have been used for many decades to model nonlinear dependencies (Aronszajn, 1950). This has found its way into nonparametric spline models (Wahba, 1990) and kernel methods (Schölkopf and Smola, 2002). It is also something that the brain solves quite naturally. After all, neurons feed into other neurons which, in turn, feed into other neurons again (Ramón y Cajal and Azoulay, 1894). Consequently we have a sequence of relatively simple transformations.

Incorporating Hidden Layers

We can overcome the limitations of linear models by incorporating one or more hidden layers. The easiest way to do this is to stack many fully connected layers on top of one another. Each layer feeds into the layer above it, until we generate outputs. We can think of the first $L - 1$ layers as our representation and the final layer as our linear predictor. This architecture is commonly called a *multilayer perceptron*, often abbreviated as *MLP* (Fig. 5.1.1).

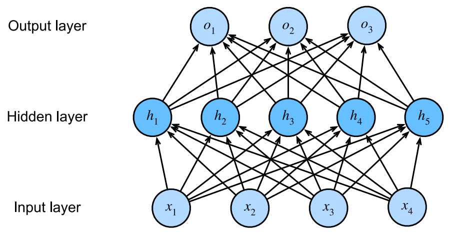


Fig. 5.1.1 An MLP with a hidden layer of five hidden units.

This MLP has four inputs, three outputs, and its hidden layer contains five hidden units. Since the input layer does not involve any calculations, producing outputs with this network requires implementing the computations for both the hidden and output layers; thus, the number of layers in this MLP is two. Note that both layers are fully connected. Every input influences every neuron in the hidden layer, and each of these in turn influences every neuron in the output layer. Alas, we are not quite done yet.

From Linear to Nonlinear

As before, we denote by the matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ a minibatch of n examples where each example has d inputs (features). For a one-hidden-layer MLP whose hidden layer has h hidden units, we denote by $\mathbf{H} \in \mathbb{R}^{n \times h}$ the outputs of the hidden layer, which are *hidden representations*. Since the hidden and output layers are both fully connected, we have hidden-layer weights $\mathbf{W}^{(1)} \in \mathbb{R}^{d \times h}$ and biases $\mathbf{b}^{(1)} \in \mathbb{R}^{1 \times h}$ and output-layer weights $\mathbf{W}^{(2)} \in \mathbb{R}^{h \times q}$ and biases $\mathbf{b}^{(2)} \in \mathbb{R}^{1 \times q}$. This allows us to calculate the outputs $\mathbf{O} \in \mathbb{R}^{n \times q}$ of the one-hidden-layer MLP as follows:

$$\begin{aligned} \mathbf{H} &= \mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)}, \\ \mathbf{O} &= \mathbf{H}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}. \end{aligned} \tag{5.1.1}$$

Note that after adding the hidden layer, our model now requires us to track and update additional sets of parameters. So what have we gained in exchange? You might be surprised to find out that—in the model defined above—*we gain nothing for our troubles*! The reason is plain. The hidden units above are given by an affine function of the inputs, and the outputs (pre-softmax) are just an affine function of the hidden units. An affine function of an affine function is itself an affine function. Moreover, our linear model was already capable of representing any affine function.

To see this formally we can just collapse out the hidden layer in the above definition, yielding an equivalent single-layer model with parameters $\mathbf{W} = \mathbf{W}^{(1)}\mathbf{W}^{(2)}$ and $\mathbf{b} = \mathbf{b}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}$:

$$\mathbf{O} = (\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})\mathbf{W}^{(2)} + \mathbf{b}^{(2)} = \mathbf{X}\mathbf{W}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)} = \mathbf{X}\mathbf{W} + \mathbf{b}. \tag{5.1.2}$$

In order to realize the potential of multilayer architectures, we need one more key ingredient: a nonlinear *activation function* σ to be applied to each hidden unit following the affine transformation. For instance, a popular choice is the ReLU (rectified linear unit) activation function (Nair and Hinton, 2010) $\sigma(x) = \max(0, x)$ operating on its arguments elementwise. The outputs of activation functions $\sigma(\cdot)$ are called *activations*. In general, with activation functions in place, it is no longer possible to collapse our MLP into a linear model:

$$\begin{aligned}\mathbf{H} &= \sigma(\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)}),\\ \mathbf{O} &= \mathbf{H}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}.\end{aligned} \tag{5.1.3}$$

Since each row in $\mathbf{X}$ corresponds to an example in the minibatch, with some abuse of notation, we define the nonlinearity σ to apply to its inputs in a rowwise fashion, i.e., one example at a time. Note that we used the same notation for softmax when we denoted a rowwise operation in Section 4.1.1. Quite frequently the activation functions we use apply not merely rowwise but elementwise. That means that after computing the linear portion of the layer, we can calculate each activation without looking at the values taken by the other hidden units.

To build more general MLPs, we can continue stacking such hidden layers, e.g., $\mathbf{H}^{(1)} = \sigma_1(\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})$ and $\mathbf{H}^{(2)} = \sigma_2(\mathbf{H}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)})$, one atop another, yielding ever more expressive models.

Universal Approximators

We know that the brain is capable of very sophisticated statistical analysis. As such, it is worth asking, just *how powerful* a deep network could be. This question has been answered multiple times, e.g., in Cybenko (1989) in the context of MLPs, and in Micchelli (1984) in the context of reproducing kernel Hilbert spaces in a way that could be seen as radial basis function (RBF) networks with a single hidden layer. These (and related results) suggest that even with a single-hidden-layer network, given enough nodes (possibly absurdly many), and the right set of weights, we can model any function. Actually learning that function is the hard part, though. You might think of your neural network as being a bit like the C programming language. The language, like any other modern language, is capable of expressing any computable program. But actually coming up with a program that meets your specifications is the hard part.

Moreover, just because a single-hidden-layer network *can* learn any function does not mean that you should try to solve all of your problems with one. In fact, in this case kernel methods are way more effective, since they are capable of solving the problem *exactly* even in infinite dimensional spaces (Kimeldorf and Wahba, 1971, Schölkopf *et al.*, 2001). In fact, we can approximate many functions much more compactly by using deeper (rather than wider) networks (Simonyan and Zisserman, 2014). We will touch upon more rigorous arguments in subsequent chapters.

5.1.2 Activation Functions

Activation functions decide whether a neuron should be activated or not by calculating the weighted sum and further adding bias to it. They are differentiable operators for transforming input signals to outputs, while most of them add nonlinearity. Because activation functions are fundamental to deep learning, let's briefly survey some common ones.

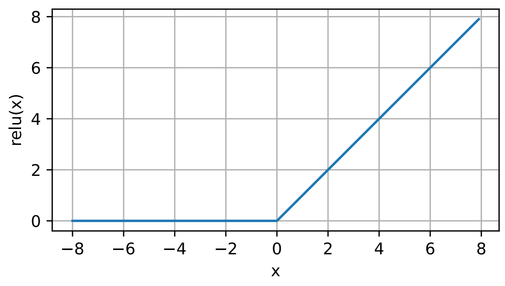
ReLU Function

The most popular choice, due to both simplicity of implementation and its good performance on a variety of predictive tasks, is the *rectified linear unit* (*ReLU*) (Nair and Hinton, 2010). ReLU provides a very simple nonlinear transformation. Given an element x, the function is defined as the maximum of that element and 0:

$$\mathrm{ReLU}(x) = \max(x, 0). \tag{5.1.4}$$

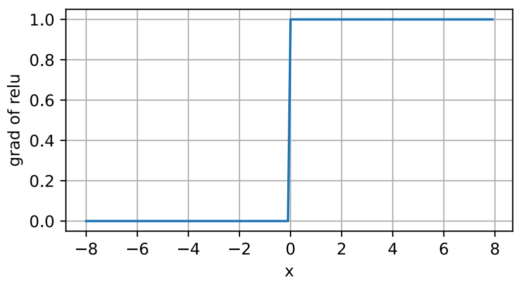
Informally, the ReLU function retains only positive elements and discards all negative elements by setting the corresponding activations to 0. To gain some intuition, we can plot the function. As you can see, the activation function is piecewise linear.

```python
x = torch.arange(-8.0, 8.0, 0.1, requires_grad=True)
y = torch.relu(x)
d2l.plot(x.detach(), y.detach(), 'x', 'relu(x)', figsize=(5, 2.5))
```



When the input is negative, the derivative of the ReLU function is 0, and when the input is positive, the derivative of the ReLU function is 1. Note that the ReLU function is not differentiable when the input takes value precisely equal to 0. In these cases, we default to the left-hand-side derivative and say that the derivative is 0 when the input is 0. We can get away with this because the input may never actually be zero (mathematicians would say that it is nondifferentiable on a set of measure zero). There is an old adage that if subtle boundary conditions matter, we are probably doing (*real*) mathematics, not engineering. That conventional wisdom may apply here, or at least, the fact that we are not performing constrained optimization (Mangasarian, 1965, Rockafellar, 1970). We plot the derivative of the ReLU function below.

```
y.backward(torch.ones_like(x), retain_graph=True)
d2l.plot(x.detach(), x.grad, 'x', 'grad of relu', figsize=(5, 2.5))
```



The reason for using ReLU is that its derivatives are particularly well behaved: either they vanish or they just let the argument through. This makes optimization better behaved and it mitigated the well-documented problem of vanishing gradients that plagued previous versions of neural networks (more on this later).

Note that there are many variants to the ReLU function, including the *parametrized ReLU* (*pReLU*) function (He *et al.*, 2015). This variation adds a linear term to ReLU, so some information still gets through, even when the argument is negative:

$$\text{pReLU}(x) = \max(0, x) + \alpha \min(0, x). \tag{5.1.5}$$

Sigmoid Function

The *sigmoid function* transforms those inputs whose values lie in the domain $\mathbb{R}$, to outputs that lie on the interval (0, 1). For that reason, the sigmoid is often called a *squashing function*: it squashes any input in the range (-inf, inf) to some value in the range (0, 1):

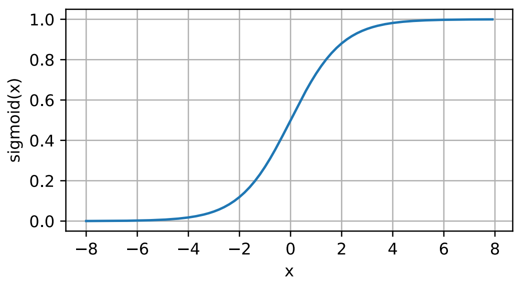
$$\text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}. \tag{5.1.6}$$

In the earliest neural networks, scientists were interested in modeling biological neurons that either *fire* or *do not fire*. Thus the pioneers of this field, going all the way back to McCulloch and Pitts, the inventors of the artificial neuron, focused on thresholding units (McCulloch and Pitts, 1943). A thresholding activation takes value 0 when its input is below some threshold and value 1 when the input exceeds the threshold.

When attention shifted to gradient-based learning, the sigmoid function was a natural choice because it is a smooth, differentiable approximation to a thresholding unit. Sigmoids are still widely used as activation functions on the output units when we want to interpret the outputs as probabilities for binary classification problems: you can think of the sigmoid as a special case of the softmax. However, the sigmoid has largely been replaced by the simpler and more easily trainable ReLU for most use in hidden layers. Much of this has to do with the fact that the sigmoid poses challenges for optimization (LeCun *et al.*, 1998) since its gradient vanishes for large positive *and* negative arguments. This can lead to plateaus that are difficult to escape from. Nonetheless sigmoids are important. In later chapters (e.g., Section 10.1) on recurrent neural networks, we will describe architectures that leverage sigmoid units to control the flow of information across time.

Below, we plot the sigmoid function. Note that when the input is close to 0, the sigmoid function approaches a linear transformation.

```
y = torch.sigmoid(x)
d2l.plot(x.detach(), y.detach(), 'x', 'sigmoid(x)', figsize=(5, 2.5))
```



The derivative of the sigmoid function is given by the following equation:

$$\frac{d}{dx}\operatorname{sigmoid}(x) = \frac{\exp(-x)}{(1+\exp(-x))^2} = \operatorname{sigmoid}(x)\left(1-\operatorname{sigmoid}(x)\right). \tag{5.1.7}$$

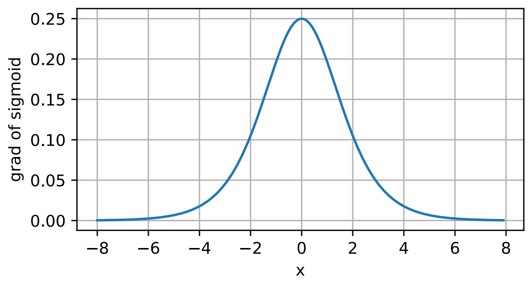
The derivative of the sigmoid function is plotted below. Note that when the input is 0, the derivative of the sigmoid function reaches a maximum of 0.25. As the input diverges from 0 in either direction, the derivative approaches 0.

```
# Clear out previous gradients
x.grad.data.zero_()
y.backward(torch.ones_like(x),retain_graph=True)
d2l.plot(x.detach(), x.grad, 'x', 'grad of sigmoid', figsize=(5, 2.5))
```

Tanh Function

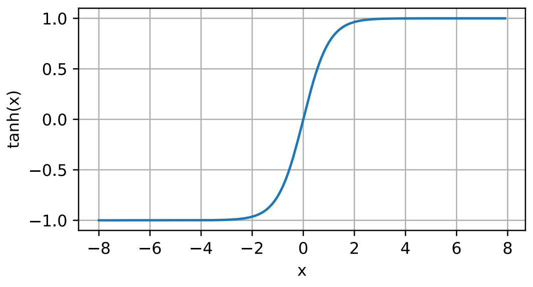
Like the sigmoid function, the tanh (hyperbolic tangent) function also squashes its inputs, transforming them into elements on the interval between -1 and 1:

$$\tanh(x) = \frac{1-\exp(-2x)}{1+\exp(-2x)}. \tag{5.1.8}$$



We plot the tanh function below. Note that as input nears 0, the tanh function approaches a linear transformation. Although the shape of the function is similar to that of the sigmoid function, the tanh function exhibits point symmetry about the origin of the coordinate system (Kalman and Kwasny, 1992).

```
y = torch.tanh(x)
d2l.plot(x.detach(), y.detach(), 'x', 'tanh(x)', figsize=(5, 2.5))
```



The derivative of the tanh function is:

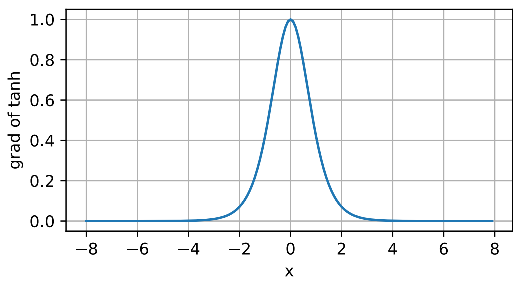
$$\frac{d}{dx}\tanh(x) = 1 - \tanh^2(x). \tag{5.1.9}$$

It is plotted below. As the input nears 0, the derivative of the tanh function approaches a maximum of 1. And as we saw with the sigmoid function, as input moves away from 0 in either direction, the derivative of the tanh function approaches 0.

```
# Clear out previous gradients
x.grad.data.zero_()
y.backward(torch.ones_like(x),retain_graph=True)
d2l.plot(x.detach(), x.grad, 'x', 'grad of tanh', figsize=(5, 2.5))
```

5.1.3 Summary and Discussion

We now know how to incorporate nonlinearities to build expressive multilayer neural network architectures. As a side note, your knowledge already puts you in command of a similar toolkit to a practitioner circa 1990. In some ways, you have an advantage over anyone



working back then, because you can leverage powerful open-source deep learning frameworks to build models rapidly, using only a few lines of code. Previously, training these networks required researchers to code up layers and derivatives explicitly in C, Fortran, or even Lisp (in the case of LeNet).

A secondary benefit is that ReLU is significantly more amenable to optimization than the sigmoid or the tanh function. One could argue that this was one of the key innovations that helped the resurgence of deep learning over the past decade. Note, though, that research in activation functions has not stopped. For instance, the GELU (Gaussian error linear unit) activation function $x\Phi(x)$ by Hendrycks and Gimpel (2016) ($\Phi(x)$ is the standard Gaussian cumulative distribution function) and the Swish activation function $\sigma(x) = x \operatorname{sigmoid}(\beta x)$ as proposed in Ramachandran *et al.* (2017) can yield better accuracy in many cases.

5.1.4 Exercises

1. Show that adding layers to a *linear* deep network, i.e., a network without nonlinearity σ can never increase the expressive power of the network. Give an example where it actively reduces it.
2. Compute the derivative of the pReLU activation function.
3. Compute the derivative of the Swish activation function $x \operatorname{sigmoid}(\beta x)$.
4. Show that an MLP using only ReLU (or pReLU) constructs a continuous piecewise linear function.
5. Sigmoid and tanh are very similar.
   1. Show that $\tanh(x) + 1 = 2 \operatorname{sigmoid}(2x)$.
   2. Prove that the function classes parametrized by both nonlinearities are identical. Hint: affine layers have bias terms, too.
6. Assume that we have a nonlinearity that applies to one minibatch at a time, such as the batch normalization (Ioffe and Szegedy, 2015). What kinds of problems do you expect this to cause?
7. Provide an example where the gradients vanish for the sigmoid activation function.

102

Discussions[102].

5.2 Implementation of Multilayer Perceptrons

Multilayer perceptrons (MLPs) are not much more complex to implement than simple linear models. The key conceptual difference is that we now concatenate multiple layers.

```
import torch
from torch import nn
from d2l import torch as d2l
```

5.2.1 Implementation from Scratch

Let's begin again by implementing such a network from scratch.

Initializing Model Parameters

Recall that Fashion-MNIST contains 10 classes, and that each image consists of a $28 \times 28 = 784$ grid of grayscale pixel values. As before we will disregard the spatial structure among the pixels for now, so we can think of this as a classification dataset with 784 input features and 10 classes. To begin, we will implement an MLP with one hidden layer and 256 hidden units. Both the number of layers and their width are adjustable (they are considered hyperparameters). Typically, we choose the layer widths to be divisible by larger powers of 2. This is computationally efficient due to the way memory is allocated and addressed in hardware.

Again, we will represent our parameters with several tensors. Note that *for every layer*, we must keep track of one weight matrix and one bias vector. As always, we allocate memory for the gradients of the loss with respect to these parameters.

In the code below we use `nn.Parameter` to automatically register a class attribute as a parameter to be tracked by `autograd` (Section 2.5).

```
class MLPScratch(d2l.Classifier):
    def __init__(self, num_inputs, num_outputs, num_hiddens, lr, sigma=0.01):
        super().__init__()
        self.save_hyperparameters()
        self.W1 = nn.Parameter(torch.randn(num_inputs, num_hiddens) * sigma)
        self.b1 = nn.Parameter(torch.zeros(num_hiddens))
        self.W2 = nn.Parameter(torch.randn(num_hiddens, num_outputs) * sigma)
        self.b2 = nn.Parameter(torch.zeros(num_outputs))
```

Model

To make sure we know how everything works, we will implement the ReLU activation ourselves rather than invoking the built-in `relu` function directly.

```
def relu(X):
    a = torch.zeros_like(X)
    return torch.max(X, a)
```

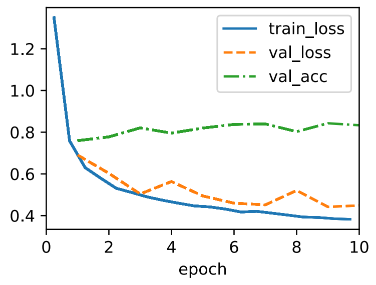
Since we are disregarding spatial structure, we `reshape` each two-dimensional image into a flat vector of length `num_inputs`. Finally, we implement our model with just a few lines of code. Since we use the framework built-in autograd this is all that it takes.

```
@d2l.add_to_class(MLPScratch)
def forward(self, X):
    X = X.reshape((-1, self.num_inputs))
    H = relu(torch.matmul(X, self.W1) + self.b1)
    return torch.matmul(H, self.W2) + self.b2
```

Training

Fortunately, the training loop for MLPs is exactly the same as for softmax regression. We define the model, data, and trainer, then finally invoke the `fit` method on model and data.

```
model = MLPScratch(num_inputs=784, num_outputs=10, num_hiddens=256, lr=0.1)
data = d2l.FashionMNIST(batch_size=256)
trainer = d2l.Trainer(max_epochs=10)
trainer.fit(model, data)
```



5.2.2 Concise Implementation

As you might expect, by relying on the high-level APIs, we can implement MLPs even more concisely.

Model

Compared with our concise implementation of softmax regression implementation (Section 4.5), the only difference is that we add *two* fully connected layers where we previously added only *one*. The first is the hidden layer, the second is the output layer.

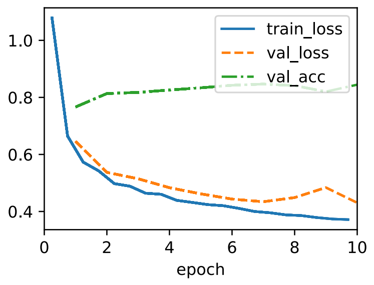
```
class MLP(d2l.Classifier):
    def __init__(self, num_outputs, num_hiddens, lr):
        super().__init__()
        self.save_hyperparameters()
        self.net = nn.Sequential(nn.Flatten(), nn.LazyLinear(num_hiddens),
                                 nn.ReLU(), nn.LazyLinear(num_outputs))
```

Previously, we defined `forward` methods for models to transform input using the model parameters. These operations are essentially a pipeline: you take an input and apply a transformation (e.g., matrix multiplication with weights followed by bias addition), then repetitively use the output of the current transformation as input to the next transformation. However, you may have noticed that no `forward` method is defined here. In fact, `MLP` inherits the `forward` method from the `Module` class (Section 3.2.2) to simply invoke `self.net(X)` (`X` is input), which is now defined as a sequence of transformations via the `Sequential` class. The `Sequential` class abstracts the forward process enabling us to focus on the transformations. We will further discuss how the `Sequential` class works in Section 6.1.2.

Training

The training loop is exactly the same as when we implemented softmax regression. This modularity enables us to separate matters concerning the model architecture from orthogonal considerations.

```
model = MLP(num_outputs=10, num_hiddens=256, lr=0.1)
trainer.fit(model, data)
```



5.2.3 Summary

Now that we have more practice in designing deep networks, the step from a single to multiple layers of deep networks does not pose such a significant challenge any longer. In particular, we can reuse the training algorithm and data loader. Note, though, that implementing MLPs from scratch is nonetheless messy: naming and keeping track of the model parameters makes it difficult to extend models. For instance, imagine wanting to insert another layer between layers 42 and 43. This might now be layer 42b, unless we are willing to perform sequential renaming. Moreover, if we implement the network from scratch, it is much more difficult for the framework to perform meaningful performance optimizations.

Nonetheless, you have now reached the state of the art of the late 1980s when fully connected deep networks were the method of choice for neural network modeling. Our next conceptual step will be to consider images. Before we do so, we need to review a number of statistical basics and details on how to compute models efficiently.

5.2.4 Exercises

1. Change the number of hidden units `num_hiddens` and plot how its number affects the accuracy of the model. What is the best value of this hyperparameter?
2. Try adding a hidden layer to see how it affects the results.
3. Why is it a bad idea to insert a hidden layer with a single neuron? What could go wrong?
4. How does changing the learning rate alter your results? With all other parameters fixed, which learning rate gives you the best results? How does this relate to the number of epochs?
5. Let's optimize over all hyperparameters jointly, i.e., learning rate, number of epochs, number of hidden layers, and number of hidden units per layer.
    1. What is the best result you can get by optimizing over all of them?
    2. Why it is much more challenging to deal with multiple hyperparameters?
    3. Describe an efficient strategy for optimizing over multiple parameters jointly.
6. Compare the speed of the framework and the from-scratch implementation for a challenging problem. How does it change with the complexity of the network?
7. Measure the speed of tensor–matrix multiplications for well-aligned and misaligned matrices. For instance, test for matrices with dimension 1024, 1025, 1026, 1028, and 1032.
    1. How does this change between GPUs and CPUs?
    2. Determine the memory bus width of your CPU and GPU.
8. Try out different activation functions. Which one works best?
9. Is there a difference between weight initializations of the network? Does it matter?

103

Discussions[103].

5.3 Forward Propagation, Backward Propagation, and Computational Graphs

So far, we have trained our models with minibatch stochastic gradient descent. However, when we implemented the algorithm, we only worried about the calculations involved in *forward propagation* through the model. When it came time to calculate the gradients, we just invoked the backpropagation function provided by the deep learning framework.

The automatic calculation of gradients profoundly simplifies the implementation of deep learning algorithms. Before automatic differentiation, even small changes to complicated models required recalculating complicated derivatives by hand. Surprisingly often, academic papers had to allocate numerous pages to deriving update rules. While we must continue to rely on automatic differentiation so we can focus on the interesting parts, you ought to know how these gradients are calculated under the hood if you want to go beyond a shallow understanding of deep learning.

In this section, we take a deep dive into the details of *backward propagation* (more commonly called *backpropagation*). To convey some insight for both the techniques and their implementations, we rely on some basic mathematics and computational graphs. To start, we focus our exposition on a one-hidden-layer MLP with weight decay (ℓ_2 regularization, to be described in subsequent chapters).

5.3.1 Forward Propagation

Forward propagation (or *forward pass*) refers to the calculation and storage of intermediate variables (including outputs) for a neural network in order from the input layer to the output layer. We now work step-by-step through the mechanics of a neural network with one hidden layer. This may seem tedious but in the eternal words of funk virtuoso James Brown, you must "pay the cost to be the boss".

For the sake of simplicity, let's assume that the input example is $\mathbf{x} \in \mathbb{R}^d$ and that our hidden layer does not include a bias term. Here the intermediate variable is:

$$\mathbf{z} = \mathbf{W}^{(1)}\mathbf{x}, \tag{5.3.1}$$

where $\mathbf{W}^{(1)} \in \mathbb{R}^{h\times d}$ is the weight parameter of the hidden layer. After running the intermediate variable $\mathbf{z} \in \mathbb{R}^h$ through the activation function ϕ we obtain our hidden activation vector of length h:

$$\mathbf{h} = \phi(\mathbf{z}). \tag{5.3.2}$$

The hidden layer output $\mathbf{h}$ is also an intermediate variable. Assuming that the parameters of the output layer possess only a weight of $\mathbf{W}^{(2)} \in \mathbb{R}^{q\times h}$, we can obtain an output layer variable with a vector of length q:

$$\mathbf{o} = \mathbf{W}^{(2)}\mathbf{h}. \tag{5.3.3}$$

Assuming that the loss function is l and the example label is y, we can then calculate the loss term for a single data example,

$$L = l(\mathbf{o}, y). \tag{5.3.4}$$

As we will see the definition of ℓ_2 regularization to be introduced later, given the hyperparameter λ, the regularization term is

$$s = \frac{\lambda}{2}\left(\|\mathbf{W}^{(1)}\|_F^2 + \|\mathbf{W}^{(2)}\|_F^2\right), \tag{5.3.5}$$

where the Frobenius norm of the matrix is simply the ℓ_2 norm applied after flattening the matrix into a vector. Finally, the model's regularized loss on a given data example is:

$$J = L + s. \tag{5.3.6}$$

We refer to J as the *objective function* in the following discussion.

5.3.2 Computational Graph of Forward Propagation

Plotting *computational graphs* helps us visualize the dependencies of operators and variables within the calculation. Fig. 5.3.1 contains the graph associated with the simple network described above, where squares denote variables and circles denote operators. The lower-left corner signifies the input and the upper-right corner is the output. Notice that the directions of the arrows (which illustrate data flow) are primarily rightward and upward.

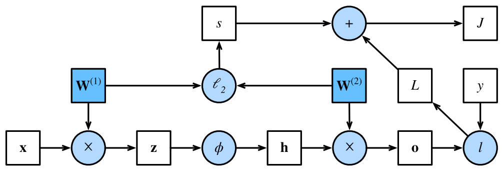


Fig. 5.3.1 Computational graph of forward propagation.

5.3.3 Backpropagation

Backpropagation refers to the method of calculating the gradient of neural network parameters. In short, the method traverses the network in reverse order, from the output to the input layer, according to the *chain rule* from calculus. The algorithm stores any intermediate variables (partial derivatives) required while calculating the gradient with respect to some parameters. Assume that we have functions $\mathsf{Y} = f(\mathsf{X})$ and $\mathsf{Z} = g(\mathsf{Y})$, in which the input and the output $\mathsf{X}, \mathsf{Y}, \mathsf{Z}$ are tensors of arbitrary shapes. By using the chain rule, we can compute the derivative of Z with respect to X via

$$\frac{\partial \mathsf{Z}}{\partial \mathsf{X}} = \text{prod}\left(\frac{\partial \mathsf{Z}}{\partial \mathsf{Y}}, \frac{\partial \mathsf{Y}}{\partial \mathsf{X}}\right). \tag{5.3.7}$$

Here we use the prod operator to multiply its arguments after the necessary operations, such as transposition and swapping input positions, have been carried out. For vectors, this is straightforward: it is simply matrix–matrix multiplication. For higher dimensional tensors, we use the appropriate counterpart. The operator prod hides all the notational overhead.

Recall that the parameters of the simple network with one hidden layer, whose computational graph is in Fig. 5.3.1, are $\mathbf{W}^{(1)}$ and $\mathbf{W}^{(2)}$. The objective of backpropagation is to calculate the gradients $\partial J/\partial \mathbf{W}^{(1)}$ and $\partial J/\partial \mathbf{W}^{(2)}$. To accomplish this, we apply the chain rule and calculate, in turn, the gradient of each intermediate variable and parameter. The order of calculations are reversed relative to those performed in forward propagation, since we need to start with the outcome of the computational graph and work our way towards the parameters. The first step is to calculate the gradients of the objective function $J = L+s$ with respect to the loss term L and the regularization term s:

$$\frac{\partial J}{\partial L} = 1 \text{ and } \frac{\partial J}{\partial s} = 1. \tag{5.3.8}$$

Next, we compute the gradient of the objective function with respect to variable of the output layer $\mathbf{o}$ according to the chain rule:

$$\frac{\partial J}{\partial \mathbf{o}} = \text{prod}\left(\frac{\partial J}{\partial L}, \frac{\partial L}{\partial \mathbf{o}}\right) = \frac{\partial L}{\partial \mathbf{o}} \in \mathbb{R}^q. \tag{5.3.9}$$

Next, we calculate the gradients of the regularization term with respect to both parameters:

$$\frac{\partial s}{\partial \mathbf{W}^{(1)}} = \lambda \mathbf{W}^{(1)} \text{ and } \frac{\partial s}{\partial \mathbf{W}^{(2)}} = \lambda \mathbf{W}^{(2)}. \tag{5.3.10}$$

Now we are able to calculate the gradient $\partial J/\partial \mathbf{W}^{(2)} \in \mathbb{R}^{q\times h}$ of the model parameters closest to the output layer. Using the chain rule yields:

$$\frac{\partial J}{\partial \mathbf{W}^{(2)}} = \text{prod}\left(\frac{\partial J}{\partial \mathbf{o}}, \frac{\partial \mathbf{o}}{\partial \mathbf{W}^{(2)}}\right) + \text{prod}\left(\frac{\partial J}{\partial s}, \frac{\partial s}{\partial \mathbf{W}^{(2)}}\right) = \frac{\partial J}{\partial \mathbf{o}} \mathbf{h}^\top + \lambda \mathbf{W}^{(2)}. \tag{5.3.11}$$

To obtain the gradient with respect to $\mathbf{W}^{(1)}$ we need to continue backpropagation along the output layer to the hidden layer. The gradient with respect to the hidden layer output $\partial J/\partial \mathbf{h} \in \mathbb{R}^h$ is given by

$$\frac{\partial J}{\partial \mathbf{h}} = \text{prod}\left(\frac{\partial J}{\partial \mathbf{o}}, \frac{\partial \mathbf{o}}{\partial \mathbf{h}}\right) = {\mathbf{W}^{(2)}}^\top \frac{\partial J}{\partial \mathbf{o}}. \tag{5.3.12}$$

Since the activation function ϕ applies elementwise, calculating the gradient $\partial J/\partial \mathbf{z} \in \mathbb{R}^h$ of the intermediate variable $\mathbf{z}$ requires that we use the elementwise multiplication operator, which we denote by $\odot$:

$$\frac{\partial J}{\partial \mathbf{z}} = \text{prod}\left(\frac{\partial J}{\partial \mathbf{h}}, \frac{\partial \mathbf{h}}{\partial \mathbf{z}}\right) = \frac{\partial J}{\partial \mathbf{h}} \odot \phi'\left(\mathbf{z}\right). \tag{5.3.13}$$

Finally, we can obtain the gradient $\partial J/\partial \mathbf{W}^{(1)} \in \mathbb{R}^{h \times d}$ of the model parameters closest to the input layer. According to the chain rule, we get

$$\frac{\partial J}{\partial \mathbf{W}^{(1)}} = \text{prod}\left(\frac{\partial J}{\partial \mathbf{z}}, \frac{\partial \mathbf{z}}{\partial \mathbf{W}^{(1)}}\right) + \text{prod}\left(\frac{\partial J}{\partial s}, \frac{\partial s}{\partial \mathbf{W}^{(1)}}\right) = \frac{\partial J}{\partial \mathbf{z}} \mathbf{x}^\top + \lambda \mathbf{W}^{(1)}. \tag{5.3.14}$$

5.3.4 Training Neural Networks

When training neural networks, forward and backward propagation depend on each other. In particular, for forward propagation, we traverse the computational graph in the direction of dependencies and compute all the variables on its path. These are then used for backpropagation where the compute order on the graph is reversed.

Take the aforementioned simple network as an illustrative example. On the one hand, computing the regularization term $(5.3.5)$ during forward propagation depends on the current values of model parameters $\mathbf{W}^{(1)}$ and $\mathbf{W}^{(2)}$. They are given by the optimization algorithm according to backpropagation in the most recent iteration. On the other hand, the gradient calculation for the parameter $(5.3.11)$ during backpropagation depends on the current value of the hidden layer output $\mathbf{h}$, which is given by forward propagation.

Therefore when training neural networks, once model parameters are initialized, we alternate forward propagation with backpropagation, updating model parameters using gradients given by backpropagation. Note that backpropagation reuses the stored intermediate values from forward propagation to avoid duplicate calculations. One of the consequences is that we need to retain the intermediate values until backpropagation is complete. This is also one of the reasons why training requires significantly more memory than plain prediction. Besides, the size of such intermediate values is roughly proportional to the number of network layers and the batch size. Thus, training deeper networks using larger batch sizes more easily leads to *out-of-memory* errors.

5.3.5 Summary

Forward propagation sequentially calculates and stores intermediate variables within the computational graph defined by the neural network. It proceeds from the input to the output layer. Backpropagation sequentially calculates and stores the gradients of intermediate variables and parameters within the neural network in the reversed order. When training deep learning models, forward propagation and backpropagation are interdependent, and training requires significantly more memory than prediction.

5.3.6 Exercises

1. Assume that the inputs $\mathbf{X}$ to some scalar function f are $n \times m$ matrices. What is the dimensionality of the gradient of f with respect to $\mathbf{X}$?
2. Add a bias to the hidden layer of the model described in this section (you do not need to include bias in the regularization term).
    1. Draw the corresponding computational graph.
    2. Derive the forward and backward propagation equations.
3. Compute the memory footprint for training and prediction in the model described in this section.
4. Assume that you want to compute second derivatives. What happens to the computational graph? How long do you expect the calculation to take?

5. Assume that the computational graph is too large for your GPU.
    1. Can you partition it over more than one GPU?
    2. What are the advantages and disadvantages over training on a smaller minibatch?

Discussions[104].

104

5.4 Numerical Stability and Initialization

Thus far, every model that we have implemented required that we initialize its parameters according to some pre-specified distribution. Until now, we took the initialization scheme for granted, glossing over the details of how these choices are made. You might have even gotten the impression that these choices are not especially important. On the contrary, the choice of initialization scheme plays a significant role in neural network learning, and it can be crucial for maintaining numerical stability. Moreover, these choices can be tied up in interesting ways with the choice of the nonlinear activation function. Which function we choose and how we initialize parameters can determine how quickly our optimization algorithm converges. Poor choices here can cause us to encounter exploding or vanishing gradients while training. In this section, we delve into these topics in greater detail and discuss some useful heuristics that you will find useful throughout your career in deep learning.

```
%matplotlib inline
import torch
from d2l import torch as d2l
```

5.4.1 Vanishing and Exploding Gradients

Consider a deep network with L layers, input $\mathbf{x}$ and output $\mathbf{o}$. With each layer l defined by a transformation f_l parametrized by weights $\mathbf{W}^{(l)}$, whose hidden layer output is $\mathbf{h}^{(l)}$ (let $\mathbf{h}^{(0)} = \mathbf{x}$), our network can be expressed as:

$$\mathbf{h}^{(l)} = f_l(\mathbf{h}^{(l-1)}) \text{ and thus } \mathbf{o} = f_L \circ \cdots \circ f_1(\mathbf{x}). \tag{5.4.1}$$

If all the hidden layer output and the input are vectors, we can write the gradient of $\mathbf{o}$ with respect to any set of parameters $\mathbf{W}^{(l)}$ as follows:

$$\partial_{\mathbf{W}^{(l)}} \mathbf{o} = \underbrace{\partial_{\mathbf{h}^{(L-1)}} \mathbf{h}^{(L)}}_{\mathbf{M}^{(L)} \stackrel{\text{def}}{=}} \cdots \underbrace{\partial_{\mathbf{h}^{(l)}} \mathbf{h}^{(l+1)}}_{\mathbf{M}^{(l+1)} \stackrel{\text{def}}{=}} \underbrace{\partial_{\mathbf{W}^{(l)}} \mathbf{h}^{(l)}}_{\mathbf{v}^{(l)} \stackrel{\text{def}}{=}}. \tag{5.4.2}$$

In other words, this gradient is the product of $L - l$ matrices $\mathbf{M}^{(L)} \cdots \mathbf{M}^{(l+1)}$ and the gradient vector $\mathbf{v}^{(l)}$. Thus we are susceptible to the same problems of numerical underflow that often crop up when multiplying together too many probabilities. When dealing with probabilities, a common trick is to switch into log-space, i.e., shifting pressure from the mantissa to the exponent of the numerical representation. Unfortunately, our problem above is more serious: initially the matrices $\mathbf{M}^{(l)}$ may have a wide variety of eigenvalues. They might be small or large, and their product might be *very large* or *very small*.

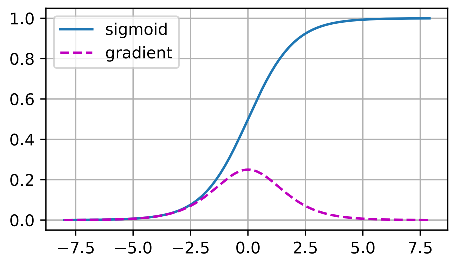
The risks posed by unstable gradients go beyond numerical representation. Gradients of unpredictable magnitude also threaten the stability of our optimization algorithms. We may be facing parameter updates that are either (i) excessively large, destroying our model (the *exploding gradient* problem); or (ii) excessively small (the *vanishing gradient* problem), rendering learning impossible as parameters hardly move on each update.

Vanishing Gradients

One frequent culprit causing the vanishing gradient problem is the choice of the activation function σ that is appended following each layer's linear operations. Historically, the sigmoid function $1/(1+\exp(-x))$ (introduced in Section 5.1) was popular because it resembles a thresholding function. Since early artificial neural networks were inspired by biological neural networks, the idea of neurons that fire either *fully* or *not at all* (like biological neurons) seemed appealing. Let's take a closer look at the sigmoid to see why it can cause vanishing gradients.

```python
x = torch.arange(-8.0, 8.0, 0.1, requires_grad=True)
y = torch.sigmoid(x)
y.backward(torch.ones_like(x))

d2l.plot(x.detach().numpy(), [y.detach().numpy(), x.grad.numpy()],
         legend=['sigmoid', 'gradient'], figsize=(4.5, 2.5))
```



As you can see, the sigmoid's gradient vanishes both when its inputs are large and when they are small. Moreover, when backpropagating through many layers, unless we are in the Goldilocks zone, where the inputs to many of the sigmoids are close to zero, the gradients of the overall product may vanish. When our network boasts many layers, unless we are careful, the gradient will likely be cut off at some layer. Indeed, this problem used to plague deep network training. Consequently, ReLUs, which are more stable (but less neurally plausible), have emerged as the default choice for practitioners.

Exploding Gradients

The opposite problem, when gradients explode, can be similarly vexing. To illustrate this a bit better, we draw 100 Gaussian random matrices and multiply them with some initial matrix. For the scale that we picked (the choice of the variance $\sigma^2 = 1$), the matrix product explodes. When this happens because of the initialization of a deep network, we have no chance of getting a gradient descent optimizer to converge.

```python
M = torch.normal(0, 1, size=(4, 4))
print('a single matrix \n',M)
for i in range(100):
    M = M @ torch.normal(0, 1, size=(4, 4))
print('after multiplying 100 matrices\n', M)
```

```
a single matrix
 tensor([[-0.8755, -1.2171,  1.3316,  0.1357],
        [ 0.4399,  1.4073, -1.9131, -0.4608],
        [-2.1420,  0.3643, -0.5267,  1.0277],
        [-0.1734, -0.7549,  2.3024,  1.3085]])
after multiplying 100 matrices
 tensor([[-2.9185e+23,  1.3915e+25, -1.1865e+25,  1.4354e+24],
        [ 4.9142e+23, -2.3430e+25,  1.9979e+25, -2.4169e+24],
        [ 2.6578e+23, -1.2672e+25,  1.0805e+25, -1.3072e+24],
        [-5.2223e+23,  2.4899e+25, -2.1231e+25,  2.5684e+24]])
```

Breaking the Symmetry

Another problem in neural network design is the symmetry inherent in their parametrization. Assume that we have a simple MLP with one hidden layer and two units. In this case, we could permute the weights $\mathbf{W}^{(1)}$ of the first layer and likewise permute the weights of the output layer to obtain the same function. There is nothing special differentiating the first and second hidden units. In other words, we have permutation symmetry among the hidden units of each layer.

This is more than just a theoretical nuisance. Consider the aforementioned one-hidden-layer MLP with two hidden units. For illustration, suppose that the output layer transforms the two hidden units into only one output unit. Imagine what would happen if we initialized all the parameters of the hidden layer as $\mathbf{W}^{(1)} = c$ for some constant c. In this case, during forward propagation either hidden unit takes the same inputs and parameters producing the same activation which is fed to the output unit. During backpropagation, differentiating the output unit with respect to parameters $\mathbf{W}^{(1)}$ gives a gradient all of whose elements take the same value. Thus, after gradient-based iteration (e.g., minibatch stochastic gradient descent), all the elements of $\mathbf{W}^{(1)}$ still take the same value. Such iterations would never *break the symmetry* on their own and we might never be able to realize the network's expressive power. The hidden layer would behave as if it had only a single unit. Note that while minibatch stochastic gradient descent would not break this symmetry, dropout regularization (to be introduced later) would!

5.4.2 Parameter Initialization

One way of addressing—or at least mitigating—the issues raised above is through careful initialization. As we will see later, additional care during optimization and suitable regularization can further enhance stability.

Default Initialization

In the previous sections, e.g., in Section 3.5, we used a normal distribution to initialize the values of our weights. If we do not specify the initialization method, the framework will use a default random initialization method, which often works well in practice for moderate problem sizes.

Xavier Initialization

Let's look at the scale distribution of an output o_i for some fully connected layer *without nonlinearities*. With $n_\textrm{in}$ inputs x_j and their associated weights w_{ij} for this layer, an output is given by

$$o_{i} = \sum_{j=1}^{n_\textrm{in}} w_{ij} x_j. \tag{5.4.3}$$

The weights w_{ij} are all drawn independently from the same distribution. Furthermore, let's assume that this distribution has zero mean and variance σ^2. Note that this does not mean that the distribution has to be Gaussian, just that the mean and variance need to exist. For now, let's assume that the inputs to the layer x_j also have zero mean and variance γ^2 and that they are independent of w_{ij} and independent of each other. In this case, we can compute the mean of o_i:

$$\begin{aligned} E[o_i] & = \sum_{j=1}^{n_\textrm{in}} E[w_{ij} x_j] \\ &= \sum_{j=1}^{n_\textrm{in}} E[w_{ij}] E[x_j] \\&= 0, \end{aligned} \tag{5.4.4}$$

and the variance:

$$\begin{aligned} \textrm{Var}[o_i] & = E[o_i^2] - (E[o_i])^2 \\ & = \sum_{j=1}^{n_\textrm{in}} E[w^2_{ij} x^2_j] - 0 \\ & = \sum_{j=1}^{n_\textrm{in}} E[w^2_{ij}] E[x^2_j] \\ & = n_\textrm{in} \sigma^2 \gamma^2. \end{aligned} \tag{5.4.5}$$

One way to keep the variance fixed is to set $n_\textrm{in} \sigma^2 = 1$. Now consider backpropagation. There we face a similar problem, albeit with gradients being propagated from the layers closer to the output. Using the same reasoning as for forward propagation, we see that the gradients' variance can blow up unless $n_{\textrm{out}}\sigma^2 = 1$, where $n_{\textrm{out}}$ is the number of outputs of this layer. This leaves us in a dilemma: we cannot possibly satisfy both conditions simultaneously. Instead, we simply try to satisfy:

$$\frac{1}{2}(n_{\textrm{in}} + n_{\textrm{out}})\sigma^2 = 1 \textrm{ or equivalently } \sigma = \sqrt{\frac{2}{n_{\textrm{in}} + n_{\textrm{out}}}}. \tag{5.4.6}$$

This is the reasoning underlying the now-standard and practically beneficial *Xavier initialization*, named after the first author of its creators (Glorot and Bengio, 2010). Typically, the Xavier initialization samples weights from a Gaussian distribution with zero mean and variance $\sigma^2 = \frac{2}{n_{\textrm{in}} + n_{\textrm{out}}}$. We can also adapt this to choose the variance when sampling weights from a uniform distribution. Note that the uniform distribution $U(-a, a)$ has variance $\frac{a^2}{3}$. Plugging $\frac{a^2}{3}$ into our condition on σ^2 prompts us to initialize according to

$$U\left(-\sqrt{\frac{6}{n_{\textrm{in}} + n_{\textrm{out}}}}, \sqrt{\frac{6}{n_{\textrm{in}} + n_{\textrm{out}}}}\right). \tag{5.4.7}$$

Though the assumption for nonexistence of nonlinearities in the above mathematical reasoning can be easily violated in neural networks, the Xavier initialization method turns out to work well in practice.

Beyond

The reasoning above barely scratches the surface of modern approaches to parameter initialization. A deep learning framework often implements over a dozen different heuristics. Moreover, parameter initialization continues to be a hot area of fundamental research in deep learning. Among these are heuristics specialized for tied (shared) parameters, super-resolution, sequence models, and other situations. For instance, Xiao *et al.* (2018) demonstrated the possibility of training 10,000-layer neural networks without architectural tricks by using a carefully-designed initialization method.

If the topic interests you we suggest a deep dive into this module's offerings, reading the papers that proposed and analyzed each heuristic, and then exploring the latest publications on the topic. Perhaps you will stumble across or even invent a clever idea and contribute an implementation to deep learning frameworks.

5.4.3 Summary

Vanishing and exploding gradients are common issues in deep networks. Great care in parameter initialization is required to ensure that gradients and parameters remain well controlled. Initialization heuristics are needed to ensure that the initial gradients are neither too large nor too small. Random initialization is key to ensuring that symmetry is broken before optimization. Xavier initialization suggests that, for each layer, variance of any output is not affected by the number of inputs, and variance of any gradient is not affected by the number of outputs. ReLU activation functions mitigate the vanishing gradient problem. This can accelerate convergence.

5.4.4 Exercises

1. Can you design other cases where a neural network might exhibit symmetry that needs breaking, besides the permutation symmetry in an MLP's layers?
2. Can we initialize all weight parameters in linear regression or in softmax regression to the same value?
3. Look up analytic bounds on the eigenvalues of the product of two matrices. What does this tell you about ensuring that gradients are well conditioned?
4. If we know that some terms diverge, can we fix this after the fact? Look at the paper on layerwise adaptive rate scaling for inspiration (You *et al.*, 2017).

Discussions[105].

105

5.5 Generalization in Deep Learning

In Chapter 3 and Chapter 4, we tackled regression and classification problems by fitting linear models to training data. In both cases, we provided practical algorithms for finding the parameters that maximized the likelihood of the observed training labels. And then, towards the end of each chapter, we recalled that fitting the training data was only an intermediate goal. Our real quest all along was to discover *general patterns* on the basis of which we can make accurate predictions even on new examples drawn from the same underlying population. Machine learning researchers are *consumers* of optimization algorithms. Sometimes, we must even develop new optimization algorithms. But at the end of the day, optimization is merely a means to an end. At its core, machine learning is a statistical discipline and we wish to optimize training loss only insofar as some statistical principle (known or unknown) leads the resulting models to generalize beyond the training set.

On the bright side, it turns out that deep neural networks trained by stochastic gradient descent generalize remarkably well across myriad prediction problems, spanning computer vision; natural language processing; time series data; recommender systems; electronic health records; protein folding; value function approximation in video games and board games; and numerous other domains. On the downside, if you were looking for a straightforward account of either the optimization story (why we can fit them to training data) or the generalization story (why the resulting models generalize to unseen examples), then you might want to pour yourself a drink. While our procedures for optimizing linear models and the statistical properties of the solutions are both described well by a comprehensive body of theory, our understanding of deep learning still resembles the wild west on both fronts.

Both the theory and practice of deep learning are rapidly evolving, with theorists adopting new strategies to explain what's going on, even as practitioners continue to innovate at a blistering pace, building arsenals of heuristics for training deep networks and a body of intuitions and folk knowledge that provide guidance for deciding which techniques to apply in which situations.

The summary of the present moment is that the theory of deep learning has produced promising lines of attack and scattered fascinating results, but still appears far from a comprehensive account of both (i) why we are able to optimize neural networks and (ii) how models learned by gradient descent manage to generalize so well, even on high-dimensional tasks. However, in practice, (i) is seldom a problem (we can always find parameters that will fit all of our training data) and thus understanding generalization is far the bigger problem. On the other hand, even absent the comfort of a coherent scientific theory, practitioners have developed a large collection of techniques that may help you to produce models that generalize well in practice. While no pithy summary can possibly do justice to the vast topic of generalization in deep learning, and while the overall state of research is far from resolved, we hope, in this section, to present a broad overview of the state of research and practice.

5.5.1 Revisiting Overfitting and Regularization

According to the "no free lunch" theorem of Wolpert and Macready (1995), any learning algorithm generalizes better on data with certain distributions, and worse with other distributions. Thus, given a finite training set, a model relies on certain assumptions: to achieve human-level performance it may be useful to identify *inductive biases* that reflect how humans think about the world. Such inductive biases show preferences for solutions with certain properties. For example, a deep MLP has an inductive bias towards building up a complicated function by the composition of simpler functions.

With machine learning models encoding inductive biases, our approach to training them typically consists of two phases: (i) fit the training data; and (ii) estimate the *generalization error* (the true error on the underlying population) by evaluating the model on holdout data. The difference between our fit on the training data and our fit on the test data is called the *generalization gap* and when this is large, we say that our models *overfit* to the training data. In extreme cases of overfitting, we might exactly fit the training data, even when the test error remains significant. And in the classical view, the interpretation is that our models are too complex, requiring that we either shrink the number of features, the number of nonzero parameters learned, or the size of the parameters as quantified. Recall the plot of model complexity compared with loss (Fig. 3.6.1) from Section 3.6.

However deep learning complicates this picture in counterintuitive ways. First, for classification problems, our models are typically expressive enough to perfectly fit every training example, even in datasets consisting of millions (Zhang *et al.*, 2021). In the classical picture, we might think that this setting lies on the far right extreme of the model complexity axis, and that any improvements in generalization error must come by way of regularization, either by reducing the complexity of the model class, or by applying a penalty, severely constraining the set of values that our parameters might take. But that is where things start to get weird.

Strangely, for many deep learning tasks (e.g., image recognition and text classification) we are typically choosing among model architectures, all of which can achieve arbitrarily low training loss (and zero training error). Because all models under consideration achieve zero training error, *the only avenue for further gains is to reduce overfitting*. Even stranger, it is often the case that despite fitting the training data perfectly, we can actually *reduce the generalization error* further by making the model *even more expressive*, e.g., adding layers, nodes, or training for a larger number of epochs. Stranger yet, the pattern relating the generalization gap to the *complexity* of the model (as captured, for example, in the depth or width of the networks) can be non-monotonic, with greater complexity hurting at first but subsequently helping in a so-called "double-descent" pattern (Nakkiran *et al.*, 2021). Thus the deep learning practitioner possesses a bag of tricks, some of which seemingly restrict the model in some fashion and others that seemingly make it even more expressive, and all of which, in some sense, are applied to mitigate overfitting.

Complicating things even further, while the guarantees provided by classical learning theory can be conservative even for classical models, they appear powerless to explain why it is that deep neural networks generalize in the first place. Because deep neural networks are capable of fitting arbitrary labels even for large datasets, and despite the use of familiar methods such as ℓ_2 regularization, traditional complexity-based generalization bounds, e.g., those based on the VC dimension or Rademacher complexity of a hypothesis class cannot explain why neural networks generalize.

5.5.2 Inspiration from Nonparametrics

Approaching deep learning for the first time, it is tempting to think of them as parametric models. After all, the models *do* have millions of parameters. When we update the models, we update their parameters. When we save the models, we write their parameters to disk. However, mathematics and computer science are riddled with counterintuitive changes of perspective, and surprising isomorphisms between seemingly different problems. While neural networks clearly *have* parameters, in some ways it can be more fruitful to think of them as behaving like nonparametric models. So what precisely makes a model nonparametric? While the name covers a diverse set of approaches, one common theme is that nonparametric methods tend to have a level of complexity that grows as the amount of available data grows.

Perhaps the simplest example of a nonparametric model is the k-nearest neighbor algorithm (we will cover more nonparametric models later, for example in Section 11.2). Here, at training time, the learner simply memorizes the dataset. Then, at prediction time, when confronted with a new point $\mathbf{x}$, the learner looks up the k nearest neighbors (the k points $\mathbf{x}_i'$ that minimize some distance $d(\mathbf{x}, \mathbf{x}_i')$). When $k = 1$, this algorithm is called 1-nearest neighbors, and the algorithm will always achieve a training error of zero. That however, does not mean that the algorithm will not generalize. In fact, it turns out that under some mild conditions, the 1-nearest neighbor algorithm is consistent (eventually converging to the optimal predictor).

Note that 1-nearest neighbor requires that we specify some distance function d, or equivalently, that we specify some vector-valued basis function $\phi(\mathbf{x})$ for featurizing our data. For any choice of the distance metric, we will achieve zero training error and eventually reach an optimal predictor, but different distance metrics d encode different inductive biases and with a finite amount of available data will yield different predictors. Different choices of the distance metric d represent different assumptions about the underlying patterns and the performance of the different predictors will depend on how compatible the assumptions are with the observed data.

In a sense, because neural networks are over-parametrized, possessing many more parameters than are needed to fit the training data, they tend to *interpolate* the training data (fitting it perfectly) and thus behave, in some ways, more like nonparametric models. More recent theoretical research has established deep connection between large neural networks and nonparametric methods, notably kernel methods. In particular, Jacot *et al.* (2018) demonstrated that in the limit, as multilayer perceptrons with randomly initialized weights grow infinitely wide, they become equivalent to (nonparametric) kernel methods for a specific choice of the kernel function (essentially, a distance function), which they call the neural tangent kernel. While current neural tangent kernel models may not fully explain the behavior of modern deep networks, their success as an analytical tool underscores the usefulness of nonparametric modeling for understanding the behavior of over-parametrized deep networks.

5.5.3 Early Stopping

While deep neural networks are capable of fitting arbitrary labels, even when labels are assigned incorrectly or randomly (Zhang *et al.*, 2021), this capability only emerges over many iterations of training. A new line of work (Rolnick *et al.*, 2017) has revealed that in the setting of label noise, neural networks tend to fit cleanly labeled data first and only subsequently to interpolate the mislabeled data. Moreover, it has been established that this phenomenon translates directly into a guarantee on generalization: whenever a model has fitted the cleanly labeled data but not randomly labeled examples included in the training set, it has in fact generalized (Garg *et al.*, 2021).

Together these findings help to motivate *early stopping*, a classic technique for regularizing deep neural networks. Here, rather than directly constraining the values of the weights, one constrains the number of epochs of training. The most common way to determine the stopping criterion is to monitor validation error throughout training (typically by checking once after each epoch) and to cut off training when the validation error has not decreased by more than some small amount ϵ for some number of epochs. This is sometimes called a *patience criterion*. As well as the potential to lead to better generalization in the setting of noisy labels, another benefit of early stopping is the time saved. Once the patience criterion is met, one can terminate training. For large models that might require days of training simultaneously across eight or more GPUs, well-tuned early stopping can save researchers days of time and can save their employers many thousands of dollars.

Notably, when there is no label noise and datasets are *realizable* (the classes are truly separable, e.g., distinguishing cats from dogs), early stopping tends not to lead to significant improvements in generalization. On the other hand, when there is label noise, or intrinsic variability in the label (e.g., predicting mortality among patients), early stopping is crucial. Training models until they interpolate noisy data is typically a bad idea.

5.5.4 Classical Regularization Methods for Deep Networks

In Chapter 3, we described several classical regularization techniques for constraining the complexity of our models. In particular, Section 3.7 introduced a method called weight decay, which consists of adding a regularization term to the loss function in order to penalize large values of the weights. Depending on which weight norm is penalized this technique is known either as ridge regularization (for ℓ_2 penalty) or lasso regularization (for an ℓ_1 penalty). In the classical analysis of these regularizers, they are considered as sufficiently restrictive on the values that the weights can take to prevent the model from fitting arbitrary labels.

In deep learning implementations, weight decay remains a popular tool. However, researchers have noted that typical strengths of ℓ_2 regularization are insufficient to prevent the networks from interpolating the data (Zhang *et al.*, 2021) and thus the benefits if interpreted as regularization might only make sense in combination with the early stopping criterion. Absent early stopping, it is possible that just like the number of layers or number of nodes (in deep learning) or the distance metric (in 1-nearest neighbor), these methods may lead to better generalization not because they meaningfully constrain the power of the neural network but rather because they somehow encode inductive biases that are better compatible with the patterns found in datasets of interests. Thus, classical regularizers remain popular in deep learning implementations, even if the theoretical rationale for their efficacy may be radically different.

Notably, deep learning researchers have also built on techniques first popularized in classical regularization contexts, such as adding noise to model inputs. In the next section we will introduce the famous dropout technique (invented by Srivastava *et al.* (2014)), which has become a mainstay of deep learning, even as the theoretical basis for its efficacy remains similarly mysterious.

5.5.5 Summary

Unlike classical linear models, which tend to have fewer parameters than examples, deep networks tend to be over-parametrized, and for most tasks are capable of perfectly fitting the training set. This *interpolation regime* challenges many hard fast-held intuitions. Functionally, neural networks look like parametric models. But thinking of them as nonparametric models can sometimes be a more reliable source of intuition. Because it is often the case that all deep networks under consideration are capable of fitting all of the training labels, nearly all gains must come by mitigating overfitting (closing the *generalization gap*). Paradoxically, the interventions that reduce the generalization gap sometimes appear to increase model complexity and at other times appear to decrease complexity. However, these methods seldom decrease complexity sufficiently for classical theory to explain the generalization of deep networks, and *why certain choices lead to improved generalization* remains for the most part a massive open question despite the concerted efforts of many brilliant researchers.

5.5.6 Exercises

1. In what sense do traditional complexity-based measures fail to account for generalization of deep neural networks?
2. Why might *early stopping* be considered a regularization technique?
3. How do researchers typically determine the stopping criterion?
4. What important factor seems to differentiate cases when early stopping leads to big improvements in generalization?
5. Beyond generalization, describe another benefit of early stopping.

106 Discussions[106].

5.6 Dropout

Let's think briefly about what we expect from a good predictive model. We want it to peform well on unseen data. Classical generalization theory suggests that to close the gap between train and test performance, we should aim for a simple model. Simplicity can come in the form of a small number of dimensions. We explored this when discussing the monomial basis functions of linear models in Section 3.6. Additionally, as we saw when discussing weight decay (ℓ_2 regularization) in Section 3.7, the (inverse) norm of the parameters also represents a useful measure of simplicity. Another useful notion of simplicity is smoothness, i.e., that the function should not be sensitive to small changes to its inputs. For instance, when we classify images, we would expect that adding some random noise to the pixels should be mostly harmless.

Bishop (1995) formalized this idea when he proved that training with input noise is equivalent to Tikhonov regularization. This work drew a clear mathematical connection between the requirement that a function be smooth (and thus simple), and the requirement that it be resilient to perturbations in the input.

Then, Srivastava *et al.* (2014) developed a clever idea for how to apply Bishop's idea to the internal layers of a network, too. Their idea, called *dropout*, involves injecting noise while computing each internal layer during forward propagation, and it has become a standard technique for training neural networks. The method is called *dropout* because we literally *drop out* some neurons during training. Throughout training, on each iteration, standard dropout consists of zeroing out some fraction of the nodes in each layer before calculating the subsequent layer.

To be clear, we are imposing our own narrative with the link to Bishop. The original paper on dropout offers intuition through a surprising analogy to sexual reproduction. The authors argue that neural network overfitting is characterized by a state in which each layer relies on a specific pattern of activations in the previous layer, calling this condition *co-adaptation*. Dropout, they claim, breaks up co-adaptation just as sexual reproduction is argued to break up co-adapted genes. While such an justification of this theory is certainly up for debate, the dropout technique itself has proved enduring, and various forms of dropout are implemented in most deep learning libraries.

The key challenge is how to inject this noise. One idea is to inject it in an *unbiased* manner so that the expected value of each layer—while fixing the others—equals the value it would have taken absent noise. In Bishop's work, he added Gaussian noise to the inputs to a linear model. At each training iteration, he added noise sampled from a distribution with mean zero $\epsilon \sim \mathcal{N}(0, \sigma^2)$ to the input $\mathbf{x}$, yielding a perturbed point $\mathbf{x}' = \mathbf{x} + \epsilon$. In expectation, $E[\mathbf{x}'] = \mathbf{x}$.

In standard dropout regularization, one zeros out some fraction of the nodes in each layer and then *debiases* each layer by normalizing by the fraction of nodes that were retained (not dropped out). In other words, with *dropout probability* p, each intermediate activation h is replaced by a random variable h' as follows:

$$h' = \begin{cases} 0 & \text{with probability } p \\ \frac{h}{1-p} & \text{otherwise} \end{cases} \tag{5.6.1}$$

By design, the expectation remains unchanged, i.e., $E[h'] = h$.

```
import torch
from torch import nn
from d2l import torch as d2l
```

5.6.1 Dropout in Practice

Recall the MLP with a hidden layer and five hidden units from Fig. 5.1.1. When we apply dropout to a hidden layer, zeroing out each hidden unit with probability p, the result can be viewed as a network containing only a subset of the original neurons. In Fig. 5.6.1, h_2 and h_5 are removed. Consequently, the calculation of the outputs no longer depends on h_2 or h_5 and their respective gradient also vanishes when performing backpropagation. In this way, the calculation of the output layer cannot be overly dependent on any one element of $h_1, \ldots, h_5$.

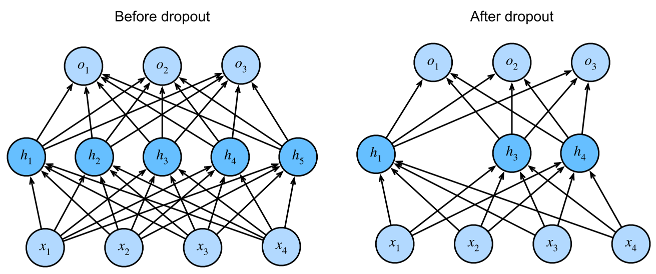


Fig. 5.6.1 MLP before and after dropout.

Typically, we disable dropout at test time. Given a trained model and a new example, we do not drop out any nodes and thus do not need to normalize. However, there are some exceptions: some researchers use dropout at test time as a heuristic for estimating the *uncertainty* of neural network predictions: if the predictions agree across many different dropout outputs, then we might say that the network is more confident.

5.6.2 Implementation from Scratch

To implement the dropout function for a single layer, we must draw as many samples from a Bernoulli (binary) random variable as our layer has dimensions, where the random variable takes value 1 (keep) with probability $1 - p$ and 0 (drop) with probability p. One easy way to implement this is to first draw samples from the uniform distribution $U[0, 1]$. Then we can keep those nodes for which the corresponding sample is greater than p, dropping the rest.

In the following code, we implement a `dropout_layer` function that drops out the elements in the tensor input `X` with probability `dropout`, rescaling the remainder as described above: dividing the survivors by `1.0-dropout`.

```python
def dropout_layer(X, dropout):
    assert 0 <= dropout <= 1
    if dropout == 1: return torch.zeros_like(X)
    mask = (torch.rand(X.shape) > dropout).float()
    return mask * X / (1.0 - dropout)
```

We can test out the `dropout_layer` function on a few examples. In the following lines of code, we pass our input `X` through the dropout operation, with probabilities 0, 0.5, and 1, respectively.

```python
X = torch.arange(16, dtype = torch.float32).reshape((2, 8))
print('dropout_p = 0:', dropout_layer(X, 0))
print('dropout_p = 0.5:', dropout_layer(X, 0.5))
print('dropout_p = 1:', dropout_layer(X, 1))
```

```
dropout_p = 0: tensor([[ 0.,  1.,  2.,  3.,  4.,  5.,  6.,  7.],
        [ 8.,  9., 10., 11., 12., 13., 14., 15.]])
dropout_p = 0.5: tensor([[ 0.,  2.,  0.,  6.,  8.,  0.,  0.,  0.],
        [16., 18., 20., 22., 24., 26., 28., 30.]])
dropout_p = 1: tensor([[0., 0., 0., 0., 0., 0., 0., 0.],
        [0., 0., 0., 0., 0., 0., 0., 0.]])
```

Defining the Model

The model below applies dropout to the output of each hidden layer (following the activation function). We can set dropout probabilities for each layer separately. A common choice is to set a lower dropout probability closer to the input layer. We ensure that dropout is only active during training.

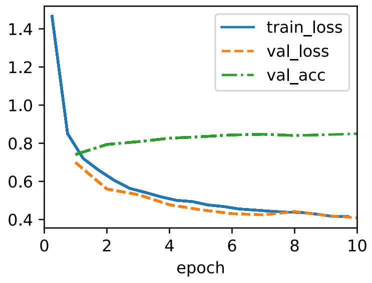
```
class DropoutMLPScratch(d2l.Classifier):
    def __init__(self, num_outputs, num_hiddens_1, num_hiddens_2,
                 dropout_1, dropout_2, lr):
        super().__init__()
        self.save_hyperparameters()
        self.lin1 = nn.LazyLinear(num_hiddens_1)
        self.lin2 = nn.LazyLinear(num_hiddens_2)
        self.lin3 = nn.LazyLinear(num_outputs)
        self.relu = nn.ReLU()

    def forward(self, X):
        H1 = self.relu(self.lin1(X.reshape((X.shape[0], -1))))
        if self.training:
            H1 = dropout_layer(H1, self.dropout_1)
        H2 = self.relu(self.lin2(H1))
        if self.training:
            H2 = dropout_layer(H2, self.dropout_2)
        return self.lin3(H2)
```

Training

The following is similar to the training of MLPs described previously.

```
hparams = {'num_outputs':10, 'num_hiddens_1':256, 'num_hiddens_2':256,
           'dropout_1':0.5, 'dropout_2':0.5, 'lr':0.1}
model = DropoutMLPScratch(**hparams)
data = d2l.FashionMNIST(batch_size=256)
trainer = d2l.Trainer(max_epochs=10)
trainer.fit(model, data)
```



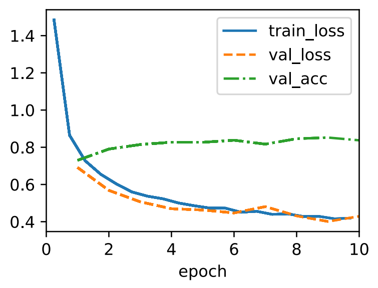
5.6.3 Concise Implementation

With high-level APIs, all we need to do is add a `Dropout` layer after each fully connected layer, passing in the dropout probability as the only argument to its constructor. During training, the `Dropout` layer will randomly drop out outputs of the previous layer (or equivalently, the inputs to the subsequent layer) according to the specified dropout probability. When not in training mode, the `Dropout` layer simply passes the data through during testing.

```
class DropoutMLP(d2l.Classifier):
    def __init__(self, num_outputs, num_hiddens_1, num_hiddens_2,
                 dropout_1, dropout_2, lr):
        super().__init__()
        self.save_hyperparameters()
        self.net = nn.Sequential(
            nn.Flatten(), nn.LazyLinear(num_hiddens_1), nn.ReLU(),
            nn.Dropout(dropout_1), nn.LazyLinear(num_hiddens_2), nn.ReLU(),
            nn.Dropout(dropout_2), nn.LazyLinear(num_outputs))
```

Next, we train the model.

```
model = DropoutMLP(**hparams)
trainer.fit(model, data)
```



5.6.4 Summary

Beyond controlling the number of dimensions and the size of the weight vector, dropout is yet another tool for avoiding overfitting. Often tools are used jointly. Note that dropout is used only during training: it replaces an activation h with a random variable with expected value h.

5.6.5 Exercises

1. What happens if you change the dropout probabilities for the first and second layers? In particular, what happens if you switch the ones for both layers? Design an experiment to answer these questions, describe your results quantitatively, and summarize the qualitative takeaways.
2. Increase the number of epochs and compare the results obtained when using dropout with those when not using it.
3. What is the variance of the activations in each hidden layer when dropout is and is not applied? Draw a plot to show how this quantity evolves over time for both models.
4. Why is dropout not typically used at test time?
5. Using the model in this section as an example, compare the effects of using dropout and

weight decay. What happens when dropout and weight decay are used at the same time? Are the results additive? Are there diminished returns (or worse)? Do they cancel each other out?

6. What happens if we apply dropout to the individual weights of the weight matrix rather than the activations?
7. Invent another technique for injecting random noise at each layer that is different from the standard dropout technique. Can you develop a method that outperforms dropout on the Fashion-MNIST dataset (for a fixed architecture)?

107 Discussions[107].

5.7 Predicting House Prices on Kaggle

Now that we have introduced some basic tools for building and training deep networks and regularizing them with techniques including weight decay and dropout, we are ready to put all this knowledge into practice by participating in a Kaggle competition. The house price prediction competition is a great place to start. The data is fairly generic and do not exhibit exotic structure that might require specialized models (as audio or video might). This dataset, collected by De Cock (2011), covers house prices in Ames, Iowa from the period 2006–2010. It is considerably larger than the famous Boston housing dataset[108] of Harrison and Rubinfeld (1978), boasting both more examples and more features.

108

In this section, we will walk you through details of data preprocessing, model design, and hyperparameter selection. We hope that through a hands-on approach, you will gain some intuitions that will guide you in your career as a data scientist.

```python
%matplotlib inline
import pandas as pd
import torch
from torch import nn
from d2l import torch as d2l
```

5.7.1 Downloading Data

Throughout the book, we will train and test models on various downloaded datasets. Here, we implement two utility functions for downloading and extracting zip or tar files. Again, we skip implementation details of such utility functions.

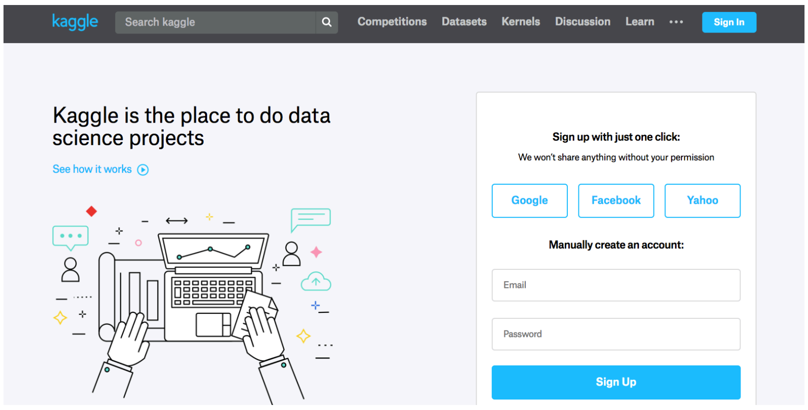
```python
def download(url, folder, sha1_hash=None):
    """Download a file to folder and return the local filepath."""

def extract(filename, folder):
    """Extract a zip/tar file into folder."""
```

5.7.2 Kaggle

109

Kaggle[109] is a popular platform that hosts machine learning competitions. Each competition centers on a dataset and many are sponsored by stakeholders who offer prizes to the winning solutions. The platform helps users to interact via forums and shared code, fostering both collaboration and competition. While leaderboard chasing often spirals out of control, with researchers focusing myopically on preprocessing steps rather than asking fundamental questions, there is also tremendous value in the objectivity of a platform that facilitates direct quantitative comparisons among competing approaches as well as code sharing so that everyone can learn what did and did not work. If you want to participate in a Kaggle competition, you will first need to register for an account (see Fig. 5.7.1).



Kaggle is the place to do data science projects

Sign up with just one click:

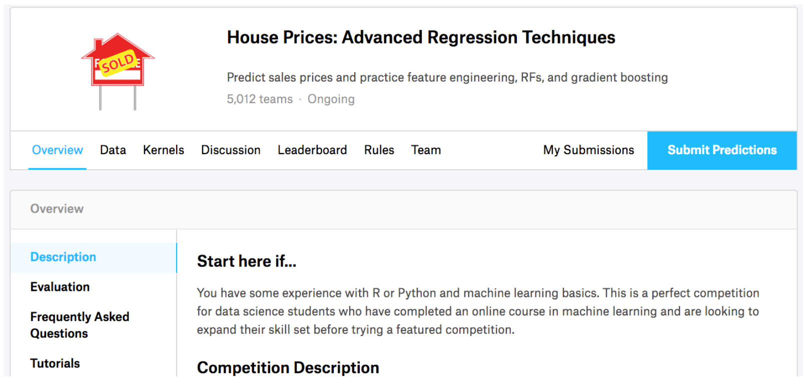
We won't share anything without your permission

Manually create an account:

Fig. 5.7.1 The Kaggle website.

On the house price prediction competition page, as illustrated in Fig. 5.7.2, you can find the dataset (under the "Data" tab), submit predictions, and see your ranking, The URL is right here:

https://www.kaggle.com/c/house-prices-advanced-regression-techniques



House Prices: Advanced Regression Techniques

Predict sales prices and practice feature engineering, RFs, and gradient boosting

5,012 teams · Ongoing

Start here if...

You have some experience with R or Python and machine learning basics. This is a perfect competition for data science students who have completed an online course in machine learning and are looking to expand their skill set before trying a featured competition.

Competition Description

Fig. 5.7.2 The house price prediction competition page.

5.7.3 Accessing and Reading the Dataset

Note that the competition data is separated into training and test sets. Each record includes the property value of the house and attributes such as street type, year of construction, roof type, basement condition, etc. The features consist of various data types. For example, the year of construction is represented by an integer, the roof type by discrete categorical assignments, and other features by floating point numbers. And here is where reality complicates things: for some examples, some data is altogether missing with the missing value marked simply as "na". The price of each house is included for the training set only (it is a competition after all). We will want to partition the training set to create a validation set, but we only get to evaluate our models on the official test set after uploading predictions to Kaggle. The "Data" tab on the competition tab in Fig. 5.7.2 has links for downloading the data.

To get started, we will read in and process the data using pandas, which we introduced in Section 2.2. For convenience, we can download and cache the Kaggle housing dataset. If a file corresponding to this dataset already exists in the cache directory and its SHA-1 matches `sha1_hash`, our code will use the cached file to avoid clogging up your Internet with redundant downloads.

```python
class KaggleHouse(d2l.DataModule):
    def __init__(self, batch_size, train=None, val=None):
        super().__init__()
        self.save_hyperparameters()
        if self.train is None:
            self.raw_train = pd.read_csv(d2l.download(
                d2l.DATA_URL + 'kaggle_house_pred_train.csv', self.root,
                sha1_hash='585e9cc93e70b39160e7921475f9bcd7d31219ce'))
            self.raw_val = pd.read_csv(d2l.download(
                d2l.DATA_URL + 'kaggle_house_pred_test.csv', self.root,
                sha1_hash='fa19780a7b011d9b009e8bff8e99922a8ee2eb90'))
```

The training dataset includes 1460 examples, 80 features, and one label, while the validation data contains 1459 examples and 80 features.

```python
data = KaggleHouse(batch_size=64)
print(data.raw_train.shape)
print(data.raw_val.shape)
```

```
Downloading ../data/kaggle_house_pred_train.csv from http://d2l-data.s3-
↪accelerate.amazonaws.com/kaggle_house_pred_train.csv...
Downloading ../data/kaggle_house_pred_test.csv from http://d2l-data.s3-
↪accelerate.amazonaws.com/kaggle_house_pred_test.csv...
(1460, 81)
(1459, 80)
```

5.7.4 Data Preprocessing

Let's take a look at the first four and final two features as well as the label (SalePrice) from the first four examples.

```python
print(data.raw_train.iloc[:4, [0, 1, 2, 3, -3, -2, -1]])
```

```
   Id  MSSubClass MSZoning  LotFrontage SaleType SaleCondition  SalePrice
0   1          60       RL         65.0       WD        Normal     208500
1   2          20       RL         80.0       WD        Normal     181500
2   3          60       RL         68.0       WD        Normal     223500
3   4          70       RL         60.0       WD       Abnorml     140000
```

We can see that in each example, the first feature is the identifier. This helps the model determine each training example. While this is convenient, it does not carry any information for prediction purposes. Hence, we will remove it from the dataset before feeding the data into the model. Furthermore, given a wide variety of data types, we will need to preprocess the data before we can start modeling.

Let's start with the numerical features. First, we apply a heuristic, replacing all missing values by the corresponding feature's mean. Then, to put all features on a common scale, we *standardize* the data by rescaling features to zero mean and unit variance:

$$x \leftarrow \frac{x - \mu}{\sigma}, \tag{5.7.1}$$

where μ and σ denote mean and standard deviation, respectively. To verify that this indeed transforms our feature (variable) such that it has zero mean and unit variance, note that $E[\frac{x-\mu}{\sigma}] = \frac{\mu-\mu}{\sigma} = 0$ and that $E[(x-\mu)^2] = (\sigma^2 + \mu^2) - 2\mu^2 + \mu^2 = \sigma^2$. Intuitively, we standardize the data for two reasons. First, it proves convenient for optimization. Second, because we do not know *a priori* which features will be relevant, we do not want to penalize coefficients assigned to one feature more than any other.

Next we deal with discrete values. These include features such as "MSZoning". We replace them by a one-hot encoding in the same way that we earlier transformed multiclass labels into vectors (see Section 4.1.1). For instance, "MSZoning" assumes the values "RL" and "RM". Dropping the "MSZoning" feature, two new indicator features "MSZoning_RL" and "MSZoning_RM" are created with values being either 0 or 1. According to one-hot encoding, if the original value of "MSZoning" is "RL", then "MSZoning_RL" is 1 and "MSZoning_RM" is 0. The `pandas` package does this automatically for us.

```python
@d2l.add_to_class(KaggleHouse)
def preprocess(self):
    # Remove the ID and label columns
    label = 'SalePrice'
    features = pd.concat(
        (self.raw_train.drop(columns=['Id', label]),
         self.raw_val.drop(columns=['Id'])))
    # Standardize numerical columns
    numeric_features = features.dtypes[features.dtypes!='object'].index
    features[numeric_features] = features[numeric_features].apply(
        lambda x: (x - x.mean()) / (x.std()))
    # Replace NAN numerical features by 0
    features[numeric_features] = features[numeric_features].fillna(0)
```

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```
    # Replace discrete features by one-hot encoding
    features = pd.get_dummies(features, dummy_na=True)
    # Save preprocessed features
    self.train = features[:self.raw_train.shape[0]].copy()
    self.train[label] = self.raw_train[label]
    self.val = features[self.raw_train.shape[0]:].copy()
```

You can see that this conversion increases the number of features from 79 to 331 (excluding ID and label columns).

```
data.preprocess()
data.train.shape
```

```
(1460, 331)
```

5.7.5 Error Measure

To get started we will train a linear model with squared loss. Not surprisingly, our linear model will not lead to a competition-winning submission but it does provide a sanity check to see whether there is meaningful information in the data. If we cannot do better than random guessing here, then there might be a good chance that we have a data processing bug. And if things work, the linear model will serve as a baseline giving us some intuition about how close the simple model gets to the best reported models, giving us a sense of how much gain we should expect from fancier models.

With house prices, as with stock prices, we care about relative quantities more than absolute quantities. Thus we tend to care more about the relative error $\frac{y-\hat{y}}{y}$ than about the absolute error $y - \hat{y}$. For instance, if our prediction is off by \$100,000 when estimating the price of a house in rural Ohio, where the value of a typical house is \$125,000, then we are probably doing a horrible job. On the other hand, if we err by this amount in Los Altos Hills, California, this might represent a stunningly accurate prediction (there, the median house price exceeds \$4 million).

One way to address this problem is to measure the discrepancy in the logarithm of the price estimates. In fact, this is also the official error measure used by the competition to evaluate the quality of submissions. After all, a small value δ for $|\log y - \log \hat{y}| \leq \delta$ translates into $e^{-\delta} \leq \frac{\hat{y}}{y} \leq e^{\delta}$. This leads to the following root-mean-squared-error between the logarithm of the predicted price and the logarithm of the label price:

$$\sqrt{\frac{1}{n}\sum_{i=1}^n\left(\log y_i - \log \hat{y}_i\right)^2}. \tag{5.7.2}$$

```
@d2l.add_to_class(KaggleHouse)
def get_dataloader(self, train):
```

(continues on next page)

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```
    label = 'SalePrice'
    data = self.train if train else self.val
    if label not in data: return
    get_tensor = lambda x: torch.tensor(x.values.astype(float),
                                  dtype=torch.float32)
    # Logarithm of prices
    tensors = (get_tensor(data.drop(columns=[label])),  # X
               torch.log(get_tensor(data[label])).reshape((-1, 1)))  # Y
    return self.get_tensorloader(tensors, train)
```

5.7.6 *K*-Fold Cross-Validation

You might recall that we introduced cross-validation in Section 3.6.3, where we discussed how to deal with model selection. We will put this to good use to select the model design and to adjust the hyperparameters. We first need a function that returns the i^{th} fold of the data in a K-fold cross-validation procedure. It proceeds by slicing out the i^{th} segment as validation data and returning the rest as training data. Note that this is not the most efficient way of handling data and we would definitely do something much smarter if our dataset was considerably larger. But this added complexity might obfuscate our code unnecessarily so we can safely omit it here owing to the simplicity of our problem.

```
def k_fold_data(data, k):
    rets = []
    fold_size = data.train.shape[0] // k
    for j in range(k):
        idx = range(j * fold_size, (j+1) * fold_size)
        rets.append(KaggleHouse(data.batch_size, data.train.drop(index=idx),
                                data.train.loc[idx]))
    return rets
```

The average validation error is returned when we train K times in the K-fold cross-validation.

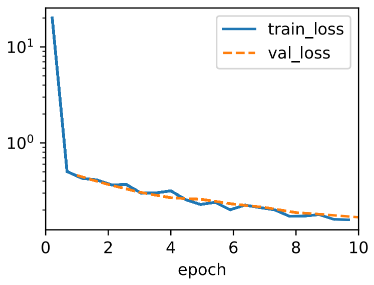
```
def k_fold(trainer, data, k, lr):
    val_loss, models = [], []
    for i, data_fold in enumerate(k_fold_data(data, k)):
        model = d2l.LinearRegression(lr)
        model.board.yscale='log'
        if i != 0: model.board.display = False
        trainer.fit(model, data_fold)
        val_loss.append(float(model.board.data['val_loss'][-1].y))
        models.append(model)
    print(f'average validation log mse = {sum(val_loss)/len(val_loss)}')
    return models
```

5.7.7 Model Selection

In this example, we pick an untuned set of hyperparameters and leave it up to the reader to improve the model. Finding a good choice can take time, depending on how many variables one optimizes over. With a large enough dataset, and the normal sorts of hyperparameters, *K*-fold cross-validation tends to be reasonably resilient against multiple testing. However, if we try an unreasonably large number of options we might find that our validation performance is no longer representative of the true error.

```
trainer = d2l.Trainer(max_epochs=10)
models = k_fold(trainer, data, k=5, lr=0.01)
```

```
average validation log mse = 0.17325432986021042
```



Notice that sometimes the number of training errors for a set of hyperparameters can be very low, even as the number of errors on *K*-fold cross-validation grows considerably higher. This indicates that we are overfitting. Throughout training you will want to monitor both numbers. Less overfitting might indicate that our data can support a more powerful model. Massive overfitting might suggest that we can gain by incorporating regularization techniques.

5.7.8 Submitting Predictions on Kaggle

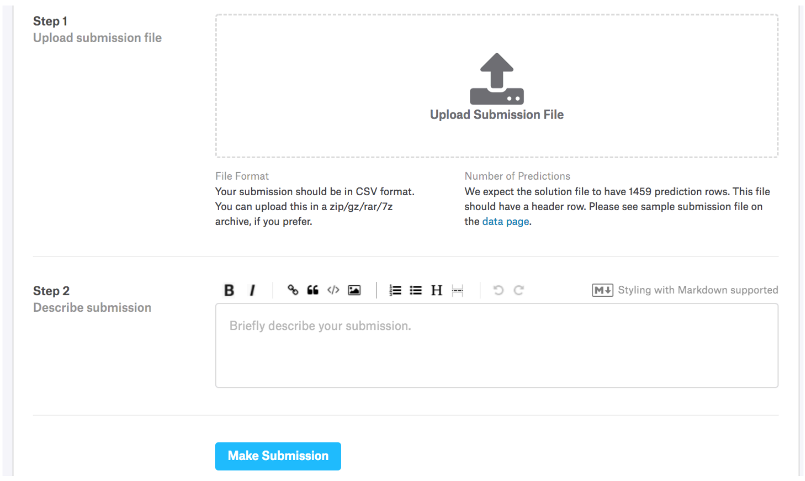
Now that we know what a good choice of hyperparameters should be, we might calculate the average predictions on the test set by all the *K* models. Saving the predictions in a csv file will simplify uploading the results to Kaggle. The following code will generate a file called `submission.csv`.

```
preds = [model(torch.tensor(data.val.values.astype(float), dtype=torch.
↪float32))
         for model in models]
# Taking exponentiation of predictions in the logarithm scale
ensemble_preds = torch.exp(torch.cat(preds, 1)).mean(1)
submission = pd.DataFrame({'Id':data.raw_val.Id,
                           'SalePrice':ensemble_preds.detach().numpy()})
submission.to_csv('submission.csv', index=False)
```

Next, as demonstrated in Fig. 5.7.3, we can submit our predictions on Kaggle and see how they compare with the actual house prices (labels) on the test set. The steps are quite simple:

- Log in to the Kaggle website and visit the house price prediction competition page.

- Click the “Submit Predictions” or “Late Submission” button.
- Click the “Upload Submission File” button in the dashed box at the bottom of the page and select the prediction file you wish to upload.
- Click the “Make Submission” button at the bottom of the page to view your results.



File Format
Your submission should be in CSV format. You can upload this in a zip/gz/rar/7z archive, if you prefer.

Number of Predictions
We expect the solution file to have 1459 prediction rows. This file should have a header row. Please see sample submission file on the data page.

Briefly describe your submission.

Fig. 5.7.3 Submitting data to Kaggle

5.7.9 Summary and Discussion

Real data often contains a mix of different data types and needs to be preprocessed. Rescaling real-valued data to zero mean and unit variance is a good default. So is replacing missing values with their mean. Furthermore, transforming categorical features into indicator features allows us to treat them like one-hot vectors. When we tend to care more about the relative error than about the absolute error, we can measure the discrepancy in the logarithm of the prediction. To select the model and adjust the hyperparameters, we can use K-fold cross-validation .

5.7.10 Exercises

1. Submit your predictions for this section to Kaggle. How good are they?
2. Is it always a good idea to replace missing values by a mean? Hint: can you construct a situation where the values are not missing at random?
3. Improve the score by tuning the hyperparameters through K-fold cross-validation.
4. Improve the score by improving the model (e.g., layers, weight decay, and dropout).
5. What happens if we do not standardize the continuous numerical features as we have done in this section?

110

Discussions[110].