Using convolutions to generalize

This chapter covers

- Understanding convolution
- Building a convolutional neural network
- Creating custom nn.Module subclasses
- The difference between the module and functional APIs
- Design choices for neural networks

In the previous chapter, we built a simple neural network that could fit (or overfit) the data, thanks to the many parameters available for optimization in the linear layers. We had issues with our model, however, in that it was better at memorizing the training set than it was at generalizing properties of birds and airplanes. Based on our model architecture, we've got a guess as to why that's the case. Due to the fully connected setup needed to detect the various possible translations of the bird or airplane in the image, we have both too many parameters (making it easier for the model to memorize the training set) and no position independence (making it harder to generalize). As we discussed in the last chapter, we could augment our

training data by using a wide variety of recropped images to try to force generalization, but that won't address the issue of having too many parameters.

There is a better way! It consists of replacing the dense, fully connected affine transformation in our neural network unit with a different linear operation: convolution.

8.1 The case for convolutions

Let's get to the bottom of what convolutions are and how we can use them in our neural networks. Yes, yes, we were in the middle of our quest to tell birds from airplanes, and our friend is still waiting for our solution, but this diversion is worth the extra time spent. We'll develop an intuition for this foundational concept in computer vision and then return to our problem equipped with superpowers.

In this section, we'll see how convolutions deliver locality and translation invariance. We'll do so by taking a close look at the formula defining convolutions and applying it using pen and paper—but don't worry, the gist will be in pictures, not formulas.

We said earlier that taking a 1D view of our input image and multiplying it by an n_output_features × n_input_features weight matrix, as is done in nn.Linear, means for each channel in the image, computing a weighted sum of all the pixels multiplied by a set of weights, one per output feature.

We also said that, if we want to recognize patterns corresponding to objects, like an airplane in the sky, we will likely need to look at how nearby pixels are arranged, and we will be less interested in how pixels that are far from each other appear in combination. Essentially, it doesn't matter if our image of a Spitfire has a tree or cloud or kite in the corner or not.

In order to translate this intuition into mathematical form, we could compute the weighted sum of a pixel with its immediate neighbors, rather than with all other pixels in the image. This would be equivalent to building weight matrices, one per output feature and output pixel location, in which all weights beyond a certain distance from a center pixel are zero. This will still be a weighted sum: that is, a linear operation.

8.1.1 What convolutions do

We identified one more desired property earlier: we would like these localized patterns to have an effect on the output regardless of their location in the image: that is, to be translation invariant. To achieve this goal in a matrix applied to the image-as-a-vector we used in chapter 7 would require implementing a rather complicated pattern of weights (don't worry if it is too complicated; it'll get better shortly): most of the weight matrix would be zero (for entries corresponding to input pixels too far away from the output pixel to have an influence). For other weights, we would have to find a way to keep entries in sync that correspond to the same relative position of input and output pixels. This means we would need to initialize them to the same values and ensure that all these tied weights stayed the same while the network is updated during training. This way, we would ensure that weights operate in neighborhoods to respond to local patterns, and local patterns are identified no matter where they occur in the image.



Of course, this approach is more than impractical. Fortunately, there is a readily available, local, translation-invariant linear operation on the image: a *convolution*. We can come up with a more compact description of a convolution, but what we are going to describe is exactly what we just delineated—only taken from a different angle.

Convolution, or more precisely, discrete convolution¹ (there's an analogous continuous version that we won't go into here), is defined for a 2D image as the scalar product of a weight matrix, the *kernel*, with every neighborhood in the input. Consider a 3×3 kernel (in deep learning, we typically use small kernels; we'll see why later on) as a 2D tensor

and a 1-channel, MxN image:

We can compute an element of the output image (without bias) as follows:

```
o11 = i11 * w00 + i12 * w01 + i22 * w02 +
i21 * w10 + i22 * w11 + i23 * w12 +
i31 * w20 + i32 * w21 + i33 * w22
```

Figure 8.1 shows this computation in action.

That is, we "translate" the kernel on the i11 location of the input image, and we multiply each weight by the value of the input image at the corresponding location. Thus, the output image is created by translating the kernel on all input locations and performing the weighted sum. For a multichannel image, like our RGB image, the weight matrix would be a $3 \times 3 \times 3$ matrix: one set of weights for every channel, contributing together to the output values.

Note that, just like the elements in the weight matrix of nn.Linear, the weights in the kernel are not known in advance, but they are initialized randomly and updated through backpropagation. Note also that the same kernel, and thus each weight in the kernel, is reused across the whole image. Thinking back to autograd, this means the use of each weight has a history spanning the entire image. Thus, the derivative of the loss with respect to a convolution weight includes contributions from the entire image.

¹ There is a subtle difference between PyTorch's convolution and mathematics' convolution: one argument's sign is flipped. If we were in a pedantic mood, we could call PyTorch's convolutions *discrete cross-correlations*.

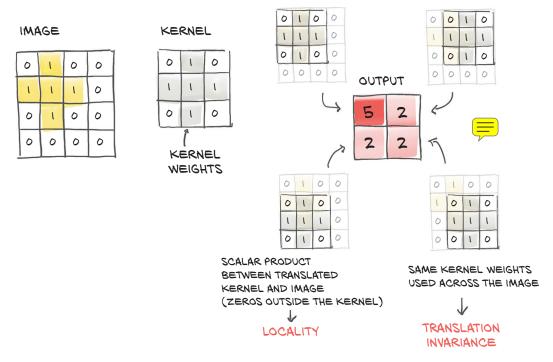


Figure 8.1 Convolution: locality and translation invariance

It's now possible to see the connection to what we were stating earlier: a convolution is equivalent to having multiple linear operations whose weights are zero almost everywhere except around individual pixels and that receive equal updates during training. Summarizing, by switching to convolutions, we get

- Local operations on neighborhoods
- Translation invariance
- Models with a lot fewer parameters

The key insight underlying the third point is that, with a convolution layer, the number of parameters depends not on the number of pixels in the image, as was the case in our fully connected model, but rather on the size of the convolution kernel $(3 \times 3, 5 \times 5, \text{ and so on})$ and on how many convolution filters (or output channels) we decide to use in our model.

8.2 Convolutions in action

Well, it looks like we've spent enough time down a rabbit hole! Let's see some PyTorch in action on our birds versus airplanes challenge. The torch.nn module provides convolutions for 1, 2, and 3 dimensions: nn.Conv1d for time series, nn.Conv2d for images, and nn.Conv3d for volumes or videos.

For our CIFAR-10 data, we'll resort to nn.Conv2d. At a minimum, the arguments we provide to nn.Conv2d are the number of input features (or *channels*, since we're dealing

with *multichannel* images: that is, more than one value per pixel), the number of output features, and the size of the kernel. For instance, for our first convolutional module, we'll have 3 input features per pixel (the RGB channels) and an arbitrary number of channels in the output—say, 16. The more channels in the output image, the more the capacity of the network. We need the channels to be able to detect many different types of features. Also, because we are randomly initializing them, some of the features we'll get, even after training, will turn out to be useless. Let's stick to a kernel size of 3×3 .

It is very common to have kernel sizes that are the same in all directions, so PyTorch has a shortcut for this: whenever kernel_size=3 is specified for a 2D convolution, it means 3×3 (provided as a tuple (3, 3) in Python). For a 3D convolution, it means $3 \times 3 \times 3$. The CT scans we will see in part 2 of the book have a different voxel (volumetric pixel) resolution in one of the three axes. In such a case, it makes sense to consider kernels that have a different size for the exceptional dimension. But for now, we stick with having the same size of convolutions across all dimensions:

```
# In[11]:

conv = nn.Conv2d(3, 16, kernel_size=3) 
conv

Instead of the shortcut kernel_size=3, we could equivalently pass in the tuple that we see in the output: kernel_size=(3, 3).

Conv2d(3, 16, kernel_size=(3, 3), stride=(1, 1))
```

What do we expect to be the shape of the weight tensor? The kernel is of size 3×3 , so we want the weight to consist of 3×3 parts. For a single output pixel value, our kernel would consider, say, in_ch = 3 input channels, so the weight component for a single output pixel value (and by translation the invariance for the entire output channel) is of shape in_ch $\times 3 \times 3$. Finally, we have as many of those as we have output channels, here out_ch = 16, so the complete weight tensor is out_ch \times in_ch \times 3 \times 3, in our case $16 \times 3 \times 3 \times 3$. The bias will have size 16 (we haven't talked about bias for a while for simplicity, but just as in the linear module case, it's a constant value we add to each channel of the output image). Let's verify our assumptions:

```
# In[12]:
conv.weight.shape, conv.bias.shape
# Out[12]:
(torch.Size([16, 3, 3, 3]), torch.Size([16]))
```

We can see how convolutions are a convenient choice for learning from images. We have smaller models looking for local patterns whose weights are optimized across the entire image.

A 2D convolution pass produces a 2D image as output, whose pixels are a weighted sum over neighborhoods of the input image. In our case, both the kernel weights and

This is part of the *lottery ticket hypothesis*: that many kernels will be as useful as losing lottery tickets. See Jonathan Frankle and Michael Carbin, "The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks," 2019, https://arxiv.org/abs/1803.03635.

the bias conv.weight are initialized randomly, so the output image will not be particularly meaningful. As usual, we need to add the zeroth batch dimension with unsqueeze if we want to call the conv module with one input image, since nn.Conv2d expects a $B \times C \times H \times W$ shaped tensor as input:

```
# In[13]:
img, _ = cifar2[0]
output = conv(img.unsqueeze(0))
img.unsqueeze(0).shape, output.shape
# Out[13]:
(torch.Size([1, 3, 32, 32]), torch.Size([1, 16, 30, 30]))
```

We're curious, so we can display the output, shown in figure 8.2:

```
# In[15]:
plt.imshow(output[0, 0].detach(), cmap='gray')
plt.show()
```

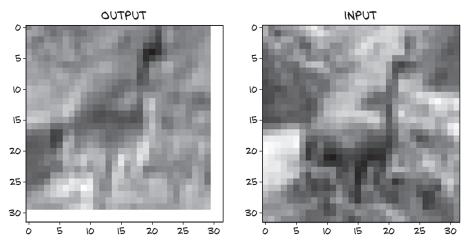


Figure 8.2 Our bird after a random convolution treatment. (We cheated a little with the code to show you the input, too.)

Wait a minute. Let's take a look a the size of output: it's torch.Size([1, 16, 30, 30]). Huh; we lost a few pixels in the process. How did that happen?

8.2.1 **Padding the boundary**

The fact that our output image is smaller than the input is a side effect of deciding what to do at the boundary of the image. Applying a convolution kernel as a weighted sum of pixels in a 3×3 neighborhood requires that there are neighbors in all directions. If we are at i00, we only have pixels to the right of and below us. By default, PyTorch will slide the convolution kernel within the input picture, getting width-kernel_width+1 horizontal and vertical positions. For odd-sized kernels, this results in images that are

199

one-half the convolution kernel's width (in our case, 3//2 = 1) smaller on each side. This explains why we're missing two pixels in each dimension.

However, PyTorch gives us the possibility of *padding* the image by creating *ghost* pixels around the border that have value zero as far as the convolution is concerned. Figure 8.3 shows padding in action.

In our case, specifying padding=1 when kernel_size=3 means i00 has an extra set of neighbors above it and to its left, so that an output of the convolution can be computed even in the corner of our original image.³ The net result is that the output has now the exact same size as the input:

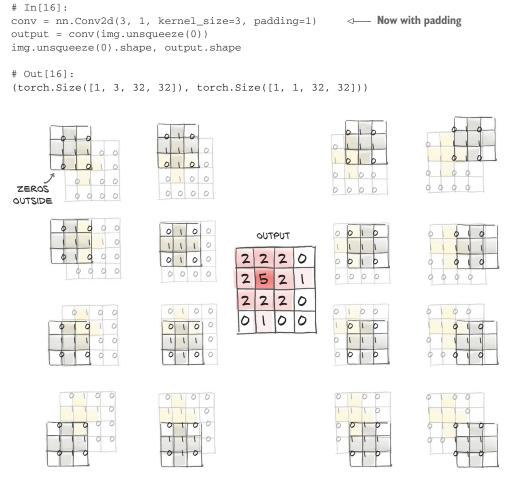


Figure 8.3 Zero padding to preserve the image size in the output

³ For even-sized kernels, we would need to pad by a different number on the left and right (and top and bottom). PyTorch doesn't offer to do this in the convolution itself, but the function torch.nn.functional .pad can take care of it. But it's best to stay with odd kernel sizes; even-sized kernels are just odd.

Note that the sizes of weight and bias don't change, regardless of whether padding is used.

There are two main reasons to pad convolutions. First, doing so helps us separate the matters of convolution and changing image sizes, we have one less thing to remember. And second, when we have more elaborate structures such as skip connections (discussed in section 8.5.3) or the U-Nets we'll cover in part 2, we want the tensors before and after a few convolutions to be of compatible size so that we can add them or take differences.

8.2.2 Detecting features with convolutions

We said earlier that weight and bias are parameters that are learned through back-propagation, exactly as it happens for weight and bias in nn. Linear. However, we can play with convolution by setting weights by hand and see what happens.

Let's first zero out bias, just to remove any confounding factors, and then set weights to a constant value so that each pixel in the output gets the mean of its neighbors. For each 3×3 neighborhood:

```
# In[17]:
with torch.no_grad():
    conv.bias.zero_()
with torch.no_grad():
    conv.weight.fill_(1.0 / 9.0)
```

We could have gone with conv.weight.one_()—that would result in each pixel in the output being the *sum* of the pixels in the neighborhood. Not a big difference, except that the values in the output image would have been nine times larger.

Anyway, let's see the effect on our CIFAR image:

```
# In[18]:
output = conv(img.unsqueeze(0))
plt.imshow(output[0, 0].detach(), cmap='gray')
plt.show()
```

As we could have predicted, the filter produces a blurred version of the image, as shown in figure 8.4. After all, every pixel of the output is the average of a neighborhood of the input, so pixels in the output are correlated and change more smoothly.

Next, let's try something different. The following kernel may look a bit mysterious at first:

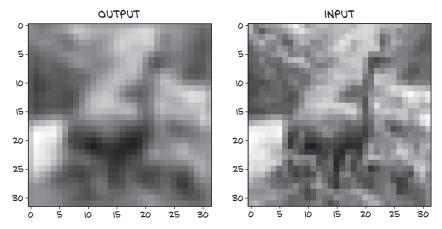


Figure 8.4 Our bird, this time blurred thanks to a constant convolution kernel

Working out the weighted sum for an arbitrary pixel in position 2,2, as we did earlier for the generic convolution kernel, we get

```
022 = i13 - i11 + i23 - i21 + i33 - i31
```

which performs the difference of all pixels on the right of i22 minus the pixels on the left of i22. If the kernel is applied on a vertical boundary between two adjacent regions of different intensity, o22 will have a high value. If the kernel is applied on a region of uniform intensity, o22 will be zero. It's an *edge-detection* kernel: the kernel highlights the vertical edge between two horizontally adjacent regions.



Applying the convolution kernel to our image, we see the result shown in figure 8.5. As expected, the convolution kernel enhances the vertical edges. We could build

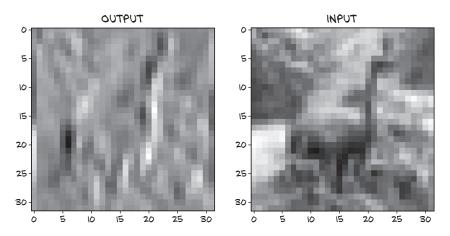


Figure 8.5 Vertical edges throughout our bird, courtesy of a handcrafted convolution kernel

lots more elaborate filters, such as for detecting horizontal or diagonal edges, or cross-like or checkerboard patterns, where "detecting" means the output has a high magnitude. In fact, the job of a computer vision expert has historically been to come up with the most effective combination of filters so that certain features are highlighted in images and objects can be recognized.

With deep learning, we let kernels be estimated from data in whatever way the discrimination is most effective: for instance, in terms of minimizing the negative cross-entropy loss between the output and the ground truth that we introduced in section 7.2.5. From this angle, the job of a convolutional neural network is to estimate the kernel of a set of filter banks in successive layers that will transform a multichannel image into another multichannel image, where different channels correspond to different features (such as one channel for the average, another channel for vertical edges, and so on). Figure 8.6 shows how the training automatically learns the kernels.

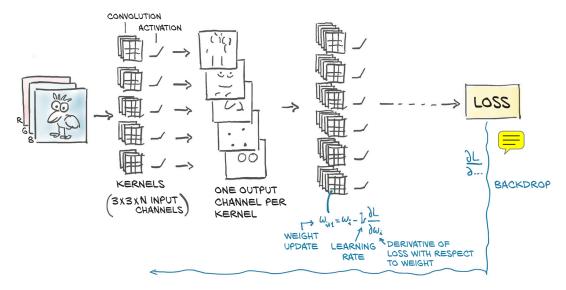


Figure 8.6 The process of learning with convolutions by estimating the gradient at the kernel weights and updating them individually in order to optimize for the loss

8.2.3 Looking further with depth and pooling

This is all well and good, but conceptually there's an elephant in the room. We got all excited because by moving from fully connected layers to convolutions, we achieve locality and translation invariance. Then we recommended the use of small kernels, like 3×3 , or 5×5 : that's peak locality, all right. What about the *big picture*? How do we know that all structures in our images are 3 pixels or 5 pixels wide? Well, we don't, because they aren't. And if they aren't, how are our networks going to be equipped to see those patterns with larger scope? This is something we'll really need if we want to

solve our birds versus airplanes problem effectively, since although CIFAR-10 images are small, the objects still have a (wing-)span several pixels across.

One possibility could be to use large convolution kernels. Well, sure, at the limit we could get a 32×32 kernel for a 32×32 image, but we would converge to the old fully connected, affine transformation and lose all the nice properties of convolution. Another option, which is used in convolutional neural networks, is stacking one convolution after the other and at the same time downsampling the image between successive convolutions.

FROM LARGE TO SMALL: DOWNSAMPLING

Downsampling could in principle occur in different ways. Scaling an image by half is the equivalent of taking four neighboring pixels as input and producing one pixel as output. How we compute the value of the output based on the values of the input is up to us. We could

- Average the four pixels. This average pooling was a common approach early on but has fallen out of favor somewhat.
- *Take the maximum of the four pixels*. This approach, called *max pooling*, is currently the most commonly used approach, but it has a downside of discarding the other three-quarters of the data.
- Perform a strided convolution, where only every Nth pixel is calculated. A 3 × 4 convolution with stride 2 still incorporates input from all pixels from the previous layer. The literature shows promise for this approach, but it has not yet supplanted max pooling.

We will be focusing on max pooling, illustrated in figure 8.7, going forward. The figure shows the most common setup of taking non-overlapping 2 x 2 tiles and taking the maximum over each of them as the new pixel at the reduced scale.

Intuitively, the output images from a convolution layer, especially since they are followed by an activation just like any other linear layer, tend to have a high magnitude

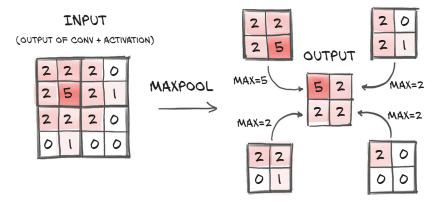


Figure 8.7 Max pooling in detail

where certain features corresponding to the estimated kernel are detected (such as vertical lines). By keeping the highest value in the 2×2 neighborhood as the downsampled output, we ensure that the features that are found *survive* the downsampling, at the expense of the weaker responses.

Max pooling is provided by the nn.MaxPool2d module (as with convolution, there are versions for 1D and 3D data). It takes as input the size of the neighborhood over which to operate the pooling operation. If we wish to downsample our image by half, we'll want to use a size of 2. Let's verify that it works as expected directly on our input image:

```
# In[21]:
pool = nn.MaxPool2d(2)
output = pool(img.unsqueeze(0))
img.unsqueeze(0).shape, output.shape
# Out[21]:
(torch.Size([1, 3, 32, 32]), torch.Size([1, 3, 16, 16]))
```

COMBINING CONVOLUTIONS AND DOWNSAMPLING FOR GREAT GOOD

Let's now see how combining convolutions and downsampling can help us recognize larger structures. In figure 8.8, we start by applying a set of 3×3 kernels on our 8×8 image, obtaining a multichannel output image of the same size. Then we scale down the output image by half, obtaining a 4×4 image, and apply another set of 3×3 kernels to it. This second set of kernels operates on a 3×3 neighborhood of something that has been scaled down by half, so it effectively maps back to 8×8 neighborhoods of the input. In addition, the second set of kernels takes the output of the first set of kernels (features like averages, edges, and so on) and extracts additional features on top of those.

So, on one hand, the first set of kernels operates on small neighborhoods on first-order, low-level features, while the second set of kernels effectively operates on wider neighborhoods, producing features that are compositions of the previous features. This is a very powerful mechanism that provides convolutional neural networks with the ability to see into very complex scenes—much more complex than our 32×32 images from the CIFAR-10 dataset.

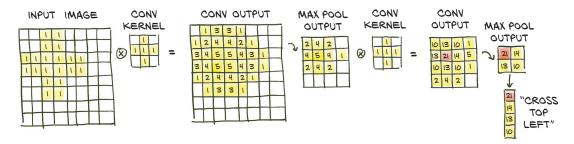


Figure 8.8 More convolutions by hand, showing the effect of stacking convolutions and downsampling: a large cross is highlighted using two small, cross-shaped kernels and max pooling.

The receptive field of output pixels

When the second 3×3 convolution kernel produces 21 in its conv output in figure 8.8, this is based on the top-left 3×3 pixels of the first max pool output. They, in turn, correspond to the 6×6 pixels in the top-left corner in the first conv output, which in turn are computed by the first convolution from the top-left 7×7 pixels. So the pixel in the second convolution output is influenced by a 7×7 input square. The first convolution also uses an implicitly "padded" column and row to produce the output in the corner; otherwise, we would have an 8×8 square of input pixels informing a given pixel (away from the boundary) in the second convolution's output. In fancy language, we say that a given output neuron of the 3×3 -conv, 2×2 -max-pool, 3×3 -conv construction has a receptive field of 8×8 .

8.2.4 Putting it all together for our network

With these building blocks in our hands, we can now proceed to build our convolutional neural network for detecting birds and airplanes. Let's take our previous fully connected model as a starting point and introduce nn.Conv2d and nn.MaxPool2d as described previously:

The first convolution takes us from 3 RGB channels to 16, thereby giving the network a chance to generate 16 independent features that operate to (hopefully) discriminate low-level features of birds and airplanes. Then we apply the Tanh activation function. The resulting 16-channel 32×32 image is pooled to a 16-channel 16×16 image by the first MaxPool3d. At this point, the downsampled image undergoes another convolution that generates an 8-channel 16×16 output. With any luck, this output will consist of higher-level features. Again, we apply a Tanh activation and then pool to an 8-channel 8×8 output.

Where does this end? After the input image has been reduced to a set of 8×8 features, we expect to be able to output some probabilities from the network that we can feed to our negative log likelihood. However, probabilities are a pair of numbers in a 1D vector (one for airplane, one for bird), but here we're still dealing with multichannel 2D features.

Thinking back to the beginning of this chapter, we already know what we need to do: turn the 8-channel 8×8 image into a 1D vector and complete our network with a set of fully connected layers:

This code gives us a neural network as shown in figure 8.9.

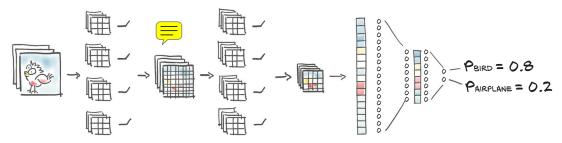


Figure 8.9 Shape of a typical convolutional network, including the one we're building. An image is fed to a series of convolutions and max pooling modules and then straightened into a 1D vector and fed into fully connected modules.

Ignore the "something missing" comment for a minute. Let's first notice that the size of the linear layer is dependent on the expected size of the output of MaxPool2d: $8 \times 8 \times 8 = 512$. Let's count the number of parameters for this small model:

```
# In[24]:
numel_list = [p.numel() for p in model.parameters()]
sum(numel_list), numel_list
# Out[24]:
(18090, [432, 16, 1152, 8, 16384, 32, 64, 2])
```

That's very reasonable for a limited dataset of such small images. In order to increase the capacity of the model, we could increase the number of output channels for the convolution layers (that is, the number of features each convolution layer generates), which would lead the linear layer to increase its size as well.

We put the "Warning" note in the code for a reason. The model has zero chance of running without complaining:

Admittedly, the error message is a bit obscure, but not too much so. We find references to linear in the traceback: looking back at the model, we see that only module that has to have a 512×32 tensor is nn.Linear (512, 32), the first linear module after the last convolution block.

What's missing there is the reshaping step from an 8-channel 8×8 image to a 512-element, 1D vector (1D if we ignore the batch dimension, that is). This could be achieved by calling view on the output of the last nn.MaxPool2d, but unfortunately, we don't have any explicit visibility of the output of each module when we use nn.Sequential.⁴



8.3 Subclassing nn. Module

At some point in developing neural networks, we will find ourselves in a situation where we want to compute something that the premade modules do not cover. Here, it is something very simple like reshaping, 5; but in section 8.5.3, we use the same construction to implement residual connections. So in this section, we learn how to make our own nn.Module subclasses that we can then use just like the prebuilt ones or nn.Sequential.

When we want to build models that do more complex things than just applying one layer after another, we need to leave nn.Sequential for something that gives us added flexibility. PyTorch allows us to use any computation in our model by subclassing nn.Module.

In order to subclass nn.Module, at a minimum we need to define a forward function that takes the inputs to the module and returns the output. This is where we define our module's computation. The name forward here is reminiscent of a distant past, when modules needed to define both the forward and backward passes we met in section 5.5.1. With PyTorch, if we use standard torch operations, autograd will take care of the backward pass automatically; and indeed, an nn.Module never comes with a backward.

Typically, our computation will use other modules—premade like convolutions or customized. To include these *submodules*, we typically define them in the constructor __init__ and assign them to self for use in the forward function. They will, at the same time, hold their parameters throughout the lifetime of our module. Note that you need to call super().__init__() before you can do that (or PyTorch will remind you).

⁴ Not being able to do this kind of operation inside of nn. Sequential was an explicit design choice by the PyTorch authors and was left that way for a long time; see the linked comments from @soumith at https://github.com/pytorch/pytorch/issues/2486. Recently, PyTorch gained an nn.Flatten layer.

⁵ We could have used nn.Flatten starting from PyTorch 1.3.

8.3.1 Our network as an nn.Module

Let's write our network as a submodule. To do so, we instantiate all the nn.Conv2d, nn.Linear, and so on that we previously passed to nn.Sequential in the constructor, and then use their instances one after another in forward:

```
# In[26]:
      class Net(nn.Module):
          def __init__(self):
              super().__init__()
               self.conv1 = nn.Conv2d(3, 16, kernel_size=3, padding=1)
               self.act1 = nn.Tanh()
               self.pool1 = nn.MaxPool2d(2)
               self.conv2 = nn.Conv2d(16, 8, kernel size=3, padding=1)
               self.act2 = nn.Tanh()
               self.pool2 = nn.MaxPool2d(2)
               self.fc1 = nn.Linear(8 * 8 * 8, 32)
               self.act3 = nn.Tanh()
               self.fc2 = nn.Linear(32, 2)
          def forward(self, x):
               out = self.pool1(self.act1(self.conv1(x)))
               out = self.pool2(self.act2(self.conv2(out)))
            → out = out.view(-1, 8 * 8 * 8)
This reshape
                                                            NET
               out = self.act3(self.fc1(out))
 is what we
               out = self.fc2(out)
were missing
```

The Net class is equivalent to the nn. Sequential model we built earlier in terms of submodules; but by writing the forward function explicitly, we can manipulate the output of self.pool3 directly and call view on it to turn it into a $B \times N$ vector. Note that we leave the batch dimension as -1 in the call to view, since in principle we don't know how many samples will be in the batch.

return out

earlier.

Here we use a subclass of nn.Module to contain our entire model. We could also use subclasses to define new building blocks for more complex networks. Picking up on the diagram style in chapter 6, our network looks like the one shown in figure 8.10. We are making some ad hoc choices about what information to present where.

Recall that the goal of classification networks typically is to compress information in the sense that we start with an image with a sizable number of pixels and compress it into (a vector of probabilities of) classes. Two things about our architecture deserve some commentary with respect to this goal.

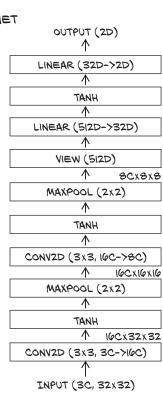


Figure 8.10 Our baseline convolutional network architecture

First, our goal is reflected by the size of our intermediate values generally shrinking—this is done by reducing the number of channels in the convolutions, by reducing the number of pixels through pooling, and by having an output dimension lower than the input dimension in the linear layers. This is a common trait of classification networks. However, in many popular architectures like the ResNets we saw in chapter 2 and discuss more in section 8.5.3, the reduction is achieved by pooling in the spatial resolution, but the number of channels increases (still resulting in a reduction in size). It seems that our pattern of fast information reduction works well with networks of limited depth and small images; but for deeper networks, the decrease is typically slower.

Second, in one layer, there is not a reduction of output size with regard to input size: the initial convolution. If we consider a single output pixel as a vector of 32 elements (the channels), it is a linear transformation of 27 elements (as a convolution of 3 channels \times 3 \times 3 kernel size)—only a moderate increase. In ResNet, the initial convolution generates 64 channels from 147 elements (3 channels \times 7 \times 7 kernel size). So the first layer is exceptional in that it greatly increases the overall dimension (as in channels times pixels) of the data flowing through it, but the mapping for each output pixel considered in isolation still has approximately as many outputs as inputs.

8.3.2 How PyTorch keeps track of parameters and submodules

Interestingly, assigning an instance of nn.Module to an attribute in an nn.Module, as we did in the earlier constructor, automatically registers the module as a submodule.

NOTE The submodules must be top-level *attributes*, not buried inside list or dict instances! Otherwise the optimizer will not be able to locate the submodules (and, hence, their parameters). For situations where your model requires a list or dict of submodules, PyTorch provides nn.ModuleList and nn.ModuleDict.

We can call arbitrary methods of an nn.Module subclass. For example, for a model where training is substantially different than its use, say, for prediction, it may make sense to have a predict method. Be aware that calling such methods will be similar to calling forward instead of the module itself—they will be ignorant of hooks, and the JIT does not see the module structure when using them because we are missing the equivalent of the __call__ bits shown in section 6.2.1.

This allows Net to have access to the parameters of its submodules without further action by the user:

⁶ The dimensions in the pixel-wise linear mapping defined by the first convolution were emphasized by Jeremy Howard in his fast.ai course (https://www.fast.ai).

⁷ Outside of and older than deep learning, projecting into high-dimensional space and then doing conceptually simpler (than linear) machine learning is commonly known as the *kernel trick*. The initial increase in the number of channels could be seen as a somewhat similar phenomenon, but striking a different balance between the cleverness of the embedding and the simplicity of the model working on the embedding.

```
# In[27]:
model = Net()

numel_list = [p.numel() for p in model.parameters()]
sum(numel_list), numel_list

# Out[27]:
(18090, [432, 16, 1152, 8, 16384, 32, 64, 2])
```

What happens here is that the parameters () call delves into all submodules assigned as attributes in the constructor and recursively calls parameters () on them. No matter how nested the submodule, any nn.Module can access the list of all child parameters. By accessing their grad attribute, which has been populated by autograd, the optimizer will know how to change parameters to minimize the loss. We know that story from chapter 5.

We now know how to implement our own modules—and we will need this a lot for part 2. Looking back at the implementation of the Net class, and thinking about the utility of registering submodules in the constructor so that we can access their parameters, it appears a bit of a waste that we are also registering submodules that have no parameters, like nn.Tanh and nn.MaxPool2d. Wouldn't it be easier to call these directly in the forward function, just as we called view?

8.3.3 The functional API

It sure would! And that's why PyTorch has *functional* counterparts for every nn module. By "functional" here we mean "having no internal state"—in other words, "whose output value is solely and fully determined by the value input arguments." Indeed, torch .nn.functional provides many functions that work like the modules we find in nn. But instead of working on the input arguments and stored parameters like the module counterparts, they take inputs and parameters as arguments to the function call. For instance, the functional counterpart of nn.Linear is nn.functional.linear, which is a function that has signature linear(input, weight, bias=None). The weight and bias parameters are arguments to the function.

Back to our model, it makes sense to keep using nn modules for nn.Linear and nn.Conv2d so that Net will be able to manage their Parameters during training. However, we can safely switch to the functional counterparts of pooling and activation, since they have no parameters:

```
# In[28]:
import torch.nn.functional as F

class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(3, 16, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(16, 8, kernel_size=3, padding=1)
        self.fc1 = nn.Linear(8 * 8 * 8, 32)
        self.fc2 = nn.Linear(32, 2)
```

```
def forward(self, x):
    out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
    out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
    out = out.view(-1, 8 * 8 * 8)
    out = torch.tanh(self.fc1(out))
    out = self.fc2(out)
    return out
```

This is a lot more concise than and fully equivalent to our previous definition of Net in section 8.3.1. Note that it would still make sense to instantiate modules that require several parameters for their initialization in the constructor.

TIP While general-purpose scientific functions like tanh still exist in torch.nn.functional in version 1.0, those entry points are deprecated in favor of functions in the top-level torch namespace. More niche functions like max pool2d will remain in torch.nn.functional.

Thus, the functional way also sheds light on what the nn.Module API is all about: a Module is a container for state in the forms of Parameters and submodules combined with the instructions to do a forward.

Whether to use the functional or the modular API is a decision based on style and taste. When part of a network is so simple that we want to use nn. Sequential, we're in the modular realm. When we are writing our own forwards, it may be more natural to use the functional interface for things that do not need state in the form of parameters.

In chapter 15, we will briefly touch on quantization. Then stateless bits like activations suddenly become stateful because information about the quantization needs to be captured. This means if we aim to quantize our model, it might be worthwhile to stick with the modular API if we go for non-JITed quantization. There is one style matter that will help you avoid surprises with (originally unforeseen) uses: if you need several applications of stateless modules (like nn.HardTanh or nn.ReLU), it is probably a good idea to have a separate instance for each. Reusing the same module appears to be clever and will give correct results with our standard Python usage here, but tools analyzing your model may trip over it.

So now we can make our own nn.Module if we need to, and we also have the functional API for cases when instantiating and then calling an nn.Module is overkill. This has been the last bit missing to understand how the code organization works in just about any neural network implemented in PyTorch.

Let's double-check that our model runs, and then we'll get to the training loop:

```
# In[29]:
model = Net()
model(img.unsqueeze(0))

# Out[29]:
tensor([[-0.0157,  0.1143]], grad_fn=<AddmmBackward>)
```

We got two numbers! Information flows correctly. We might not realize it right now, but in more complex models, getting the size of the first linear layer right is sometimes a source of frustration. We've heard stories of famous practitioners putting in arbitrary numbers and then relying on error messages from PyTorch to backtrack the correct sizes for their linear layers. Lame, eh? Nah, it's all legit!

8.4 Training our convnet

We're now at the point where we can assemble our complete training loop. We already developed the overall structure in chapter 5, and the training loop looks much like the one from chapter 6, but here we will revisit it to add some details like some tracking for accuracy. After we run our model, we will also have an appetite for a little more speed, so we will learn how to run our models fast on a GPU. But first let's look at the training loop.

Recall that the core of our convnet is two nested loops: an outer one over the *epochs* and an inner one of the DataLoader that produces batches from our Dataset. In each loop, we then have to

- 1 Feed the inputs through the model (the forward pass).
- 2 Compute the loss (also part of the forward pass).
- 3 Zero any old gradients.
- 4 Call loss.backward() to compute the gradients of the loss with respect to all parameters (the backward pass).
- 5 Have the optimizer take a step in toward lower loss.

Also, we collect and print some information. So here is our training loop, looking almost as it does in the previous chapter—but it is good to remember what each thing is doing:

```
Uses the datetime module
  included with Python
                                                                       Our loop over the epochs.
                                                                   numbered from 1 to n epochs
       # In[30]:
                                                                        rather than starting at 0
    → import datetime
       def training_loop(n_epochs, optimizer, model, loss_fn, train_loader):
           for epoch in range(1, n_epochs + 1):
                loss_train = 0.0
                                                               Loops over our dataset in
                for imgs, labels in train_loader:
                                                               the batches the data loader
 Feeds a batch
                                                               creates for us
  through our
                    outputs = model(imgs)
    model ...
                     loss = loss_fn(outputs, labels) <-</pre>
                                                                 ... and computes the loss
After getting rid of
                                                                 we wish to minimize
the gradients from poptimizer.zero_grad()
 the last round ...
                     loss.backward()
                                                    ... performs the backward step. That is, we
                                                    compute the gradients of all parameters we
                    optimizer.step()
                                                    want the network to learn.
      Updates
     the model
```

```
loss_train += loss.item()
                 if epoch == 1 or epoch % 10 == 0:
Sums the losses
                      print('{} Epoch {}, Training loss {}'.format(
we saw over the epoch.
                           datetime.datetime.now(), epoch,
                                                                         Divides by the length of the
Recall that it is important
                           loss_train / len(train_loader))) <-
                                                                        training data loader to get the
to transform the loss to a
                                                                         average loss per batch. This is a
Python number with .item(),
                                                                         much more intuitive measure than
to escape the gradients.
                                                                         the sum.
```

We use the Dataset from chapter 7; wrap it into a DataLoader; instantiate our network, an optimizer, and a loss function as before; and call our training loop.

The substantial changes in our model from the last chapter are that now our model is a custom subclass of nn.Module and that we're using convolutions. Let's run training for 100 epochs while printing the loss. Depending on your hardware, this may take 20 minutes or more to finish!

```
The DataLoader batches up the examples of our cifar2 dataset.
Shuffling randomizes the order of the examples from the dataset.
    # In[31]:
    train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                                  shuffle=True)
                                Instantiates our network ...
                                                                  ... the stochastic gradient
    model = Net() #
                                                                  descent optimizer we have
    optimizer = optim.SGD(model.parameters(), lr=1e-2)
                                                              been working with ...
    loss_fn = nn.CrossEntropyLoss() #
                                                        ... and the cross entropy
    training_loop(
                                    Calls the training
                                                       loss we met in 7.10
        n_{epochs} = 100,
                                    loop we defined
        optimizer = optimizer,
                                   earlier
        model = model,
        loss_fn = loss_fn,
        train_loader = train_loader,
    # Out[31]:
    2020-01-16 23:07:21.889707 Epoch 1, Training loss 0.5634813266954605
    2020-01-16 23:07:37.560610 Epoch 10, Training loss 0.3277610331109375
    2020-01-16 23:07:54.966180 Epoch 20, Training loss 0.3035225479086493
    2020-01-16 23:08:12.361597 Epoch 30, Training loss 0.28249378549824855
    2020-01-16 23:08:29.769820 Epoch 40, Training loss 0.2611226033253275
    2020-01-16 23:08:47.185401 Epoch 50, Training loss 0.24105800626574048
    2020-01-16 23:09:04.644522 Epoch 60, Training loss 0.21997178820477928
    2020-01-16 23:09:22.079625 Epoch 70, Training loss 0.20370126601047578
    2020-01-16 23:09:39.593780 Epoch 80, Training loss 0.18939699422401987
    2020-01-16 23:09:57.111441 Epoch 90, Training loss 0.17283396527266046
```

So now we can train our network. But again, our friend the bird watcher will likely not be impressed when we tell her that we trained to very low training loss.

2020-01-16 23:10:14.632351 Epoch 100, Training loss 0.1614033816868712

8.4.1 Measuring accuracy



In order to have a measure that is more interpretable than the loss, we can take a look at our accuracies on the training and validation datasets. We use the same code as in chapter 7:

```
# In[32]:
   train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                                   shuffle=False)
   val_loader = torch.utils.data.DataLoader(cifar2_val, batch_size=64,
                                                 shuffle=False)
   def validate(model, train_loader, val_loader):
        for name, loader in [("train", train loader), ("val", val loader)]:
            correct = 0
                                             We do not want gradients
            total = 0
                                             here, as we will not want to
                                            update the parameters.
            with torch.no_grad():
                                                                         Counts the number of
                 for imgs, labels in loader:
                                                                         examples, so total is
                     outputs = model(imgs)
Gives us the index
                                                                        increased by the batch
                  → _, predicted = torch.max(outputs, dim=1)
   of the highest
                                                                        size
                     total += labels.shape[0] <--
  value as output
                     correct += int((predicted == labels).sum())
            print("Accuracy {}: {:.2f}".format(name , correct / total))
   validate(model, train_loader, val_loader)
                                                      Comparing the predicted class that had the
                                                      maximum probability and the ground-truth
                                                    labels, we first get a Boolean array. Taking the
   # Out[32]:
                                                      sum gives the number of items in the batch
   Accuracy train: 0.93
                                                     where the prediction and ground truth agree.
   Accuracy val: 0.89
```

We cast to a Python int—for integer tensors, this is equivalent to using .item(), similar to what we did in the training loop.

This is quite a lot better than the fully connected model, which achieved only 79% accuracy. We about halved the number of errors on the validation set. Also, we used far fewer parameters. This is telling us that the model does a better job of generalizing its task of recognizing the subject of images from a new sample, through locality and translation invariance. We could now let it run for more epochs and see what performance we could squeeze out.

8.4.2 Saving and loading our model

Since we're satisfied with our model so far, it would be nice to actually save it, right? It's easy to do. Let's save the model to a file:

```
# In[33]:
torch.save(model.state_dict(), data_path + 'birds_vs_airplanes.pt')
```

The birds_vs_airplanes.pt file now contains all the parameters of model: that is, weights and biases for the two convolution modules and the two linear modules. So,

no structure—just the weights. This means when we deploy the model in production for our friend, we'll need to keep the model class handy, create an instance, and then load the parameters back into it:

| We will have to make sure we don't change

We have also included a pretrained model in our code repository, saved to ../data/p1ch7/birds_vs_airplanes.pt.

8.4.3 Training on the GPU

We have a net and can train it! But it would be good to make it a bit faster. It is no surprise by now that we do so by moving our training onto the GPU. Using the .to method we saw in chapter 3, we can move the tensors we get from the data loader to the GPU, after which our computation will automatically take place there. But we also need to move our parameters to the GPU. Happily, nn.Module implements a .to function that moves all of its parameters to the GPU (or casts the type when you pass a dtype argument).

There is a somewhat subtle difference between Module.to and Tensor.to. Module.to is in place: the module instance is modified. But Tensor.to is out of place (in some ways computation, just like Tensor.tanh), returning a new tensor. One implication is that it is good practice to create the Optimizer after moving the parameters to the appropriate device.

It is considered good style to move things to the GPU if one is available. A good pattern is to set the a variable device depending on torch.cuda.is_available:

Then we can amend the training loop by moving the tensors we get from the data loader to the GPU by using the Tensor. to method. Note that the code is exactly like our first version at the beginning of this section except for the two lines moving the inputs to the GPU:

```
# In[36]:
import datetime

def training_loop(n_epochs, optimizer, model, loss_fn, train_loader):
    for epoch in range(1, n_epochs + 1):
        loss_train = 0.0
```

```
for imgs, labels in train_loader:
    imgs = imgs.to(device=device)
                                              These two lines that move imgs and
    labels = labels.to(device=device)
                                              labels to the device we are training
    outputs = model(imas)
                                              on are the only difference from our
    loss = loss_fn(outputs, labels)
                                              previous version.
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
    loss_train += loss.item()
if epoch == 1 or epoch % 10 == 0:
    print('{} Epoch {}, Training loss {}'.format(
        datetime.datetime.now(), epoch,
        loss_train / len(train_loader)))
```

The same amendment must be made to the validate function. We can then instantiate our model, move it to device, and run it as before:⁸

```
# In[37]:
train_loader = torch.utils.data.DataLoader(cifar2, batch_size=64,
                                             shuffle=True)
model = Net().to(device=device)
                                                          Moves our model (all
optimizer = optim.SGD(model.parameters(), 1r=1e-2)
                                                          parameters) to the GPU. If
loss_fn = nn.CrossEntropyLoss()
                                                          you forget to move either the
                                                          model or the inputs to the
training_loop(
                                                          GPU, you will get errors about
    n_{epochs} = 100,
                                                          tensors not being on the same
    optimizer = optimizer,
                                                          device, because the PyTorch
    model = model,
                                                          operators do not support
                                                          mixing GPU and CPU inputs.
    loss_fn = loss_fn,
    train_loader = train_loader,
)
# Out[371:
2020-01-16 23:10:35.563216 Epoch 1, Training loss 0.5717791349265227
2020-01-16 23:10:39.730262 Epoch 10, Training loss 0.3285350770137872
2020-01-16 23:10:45.906321 Epoch 20, Training loss 0.29493294959994637
2020-01-16 23:10:52.086905 Epoch 30, Training loss 0.26962305994550134
2020-01-16 23:10:56.551582 Epoch 40, Training loss 0.24709946277794564
2020-01-16 23:11:00.991432 Epoch 50, Training loss 0.22623272664892446
2020-01-16 23:11:05.421524 Epoch 60, Training loss 0.20996672821462534
2020-01-16 23:11:09.951312 Epoch 70, Training loss 0.1934866009719053
2020-01-16 23:11:14.499484 Epoch 80, Training loss 0.1799132404908253
2020-01-16 23:11:19.047609 Epoch 90, Training loss 0.16620008706761774
2020-01-16 23:11:23.590435 Epoch 100, Training loss 0.15667157247662544
```

⁸ There is a pin_memory option for the data loader that will cause the data loader to use memory pinned to the GPU, with the goal of speeding up transfers. Whether we gain something varies, though, so we will not pursue this here.

Even for our small network here, we do see a sizable increase in speed. The advantage of computing on GPUs is more visible for larger models.

There is a slight complication when loading network weights: PyTorch will attempt to load the weight to the same device it was saved from—that is, weights on the GPU will be restored to the GPU. As we don't know whether we want the same device, we have two options: we could move the network to the CPU before saving it, or move it back after restoring. It is a bit more concise to instruct PyTorch to override the device information when loading weights. This is done by passing the map_location keyword argument to torch.load:

8.5 Model design

We built our model as a subclass of nn.Module, the de facto standard for all but the simplest models. Then we trained it successfully and saw how to use the GPU to train our models. We've reached the point where we can build a feed-forward convolutional neural network and train it successfully to classify images. The natural question is, what now? What if we are presented with a more complicated problem? Admittedly, our birds versus airplanes dataset wasn't that complicated: the images were very small, and the object under investigation was centered and took up most of the viewport.



If we moved to, say, ImageNet, we would find larger, more complex images, where the right answer would depend on multiple visual clues, often hierarchically organized. For instance, when trying to predict whether a dark brick shape is a remote control or a cell phone, the network could be looking for something like a screen.

Plus images may not be our sole focus in the real world, where we have tabular data, sequences, and text. The promise of neural networks is sufficient flexibility to solve problems on all these kinds of data given the proper architecture (that is, the interconnection of layers or modules) and the proper loss function.

PyTorch ships with a very comprehensive collection of modules and loss functions to implement state-of-the-art architectures ranging from feed-forward components to long short-term memory (LSTM) modules and transformer networks (two very popular architectures for sequential data). Several models are available through PyTorch Hub or as part of torchvision and other vertical community efforts.

We'll see a few more advanced architectures in part 2, where we'll walk through an end-to-end problem of analyzing CT scans, but in general, it is beyond the scope of this book to explore variations on neural network architectures. However, we can build on the knowledge we've accumulated thus far to understand how we can implement



almost any architecture thanks to the expressivity of PyTorch. The purpose of this section is precisely to provide conceptual tools that will allow us to read the latest research paper and start implementing it in PyTorch—or, since authors often release PyTorch implementations of their papers, to read the implementations without choking on our coffee.

8.5.1 Adding memory capacity: Width

Given our feed-forward architecture, there are a couple of dimensions we'd likely want to explore before getting into further complications. The first dimension is the *width* of the network: the number of neurons per layer, or channels per convolution. We can make a model wider very easily in PyTorch. We just specify a larger number of output channels in the first convolution and increase the subsequent layers accordingly, taking care to change the forward function to reflect the fact that we'll now have a longer vector once we switch to fully connected layers:

```
# In[40]:
class NetWidth(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(3, 32, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(32, 16, kernel_size=3, padding=1)
        self.fc1 = nn.Linear(16 * 8 * 8, 32)
        self.fc2 = nn.Linear(32, 2)

def forward(self, x):
    out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
    out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
    out = out.view(-1, 16 * 8 * 8)
    out = torch.tanh(self.fc1(out))
    out = self.fc2(out)
    return out
```

If we want to avoid hardcoding numbers in the definition of the model, we can easily pass a parameter to *init* and parameterize the width, taking care to also parameterize the call to view in the forward function:

```
# In[42]:
class NetWidth(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3, padding=1)
        self.fc1 = nn.Linear(8 * 8 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)

def forward(self, x):
        out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
        out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
```

```
out = out.view(-1, 8 * 8 * self.n_chans1 // 2)
out = torch.tanh(self.fc1(out))
out = self.fc2(out)
return out
```

The numbers specifying channels and features for each layer are directly related to the number of parameters in a model; all other things being equal, they increase the *capacity* of the model. As we did previously, we can look at how many parameters our model has now:

```
# In[44]:
sum(p.numel() for p in model.parameters())
# Out[44]:
38386
```

The greater the capacity, the more variability in the inputs the model will be able to manage; but at the same time, the more likely overfitting will be, since the model can use a greater number of parameters to memorize unessential aspects of the input. We already went into ways to combat overfitting, the best being increasing the sample size or, in the absence of new data, augmenting existing data through artificial modifications of the same data.

There are a few more tricks we can play at the model level (without acting on the data) to control overfitting. Let's review the most common ones.

8.5.2 Helping our model to converge and generalize: Regularization

Training a model involves two critical steps: optimization, when we need the loss to decrease on the training set; and generalization, when the model has to work not only on the training set but also on data it has not seen before, like the validation set. The mathematical tools aimed at easing these two steps are sometimes subsumed under the label *regularization*.

KEEPING THE PARAMETERS IN CHECK: WEIGHT PENALTIES

The first way to stabilize generalization is to add a regularization term to the loss. This term is crafted so that the weights of the model tend to be small on their own, limiting how much training makes them grow. In other words, it a penalty on larger weight values. This makes the loss have a smoother topography, and there's relatively less to gain from fitting individual samples.

The most popular regularization terms of this kind are L2 regularization, which is the sum of squares of all weights in the model, and L1 regularization, which is the sum of the absolute values of all weights in the model.⁹ Both of them are scaled by a (small) factor, which is a hyperparameter we set prior to training.

⁹ We'll focus on L2 regularization here. L1 regularization—popularized in the more general statistics literature by its use in Lasso—has the attractive property of resulting in sparse trained weights.

L2 regularization is also referred to as weight decay. The reason for this name is that, thinking about SGD and backpropagation, the negative gradient of the L2 regularization term with respect to a parameter w_i is - 2 * lambda * w_i, where lambda is the aforementioned hyperparameter, simply named weight decay in PyTorch. So, adding L2 regularization to the loss function is equivalent to decreasing each weight by an amount proportional to its current value during the optimization step (hence, the name weight decay). Note that weight decay applies to all parameters of the network, such as biases.

In PyTorch, we could implement regularization pretty easily by adding a term to the loss. After computing the loss, whatever the loss function is, we can iterate the parameters of the model, sum their respective square (for L2) or abs (for L1), and backpropagate:

```
# In[45]:
def training_loop_l2reg(n_epochs, optimizer, model, loss_fn,
                         train_loader):
    for epoch in range(1, n_epochs + 1):
        loss_train = 0.0
        for imgs, labels in train_loader:
            imgs = imgs.to(device=device)
            labels = labels.to(device=device)
            outputs = model(imgs)
            loss = loss_fn(outputs, labels)
            12_{\text{lambda}} = 0.001
                                                                 Replaces pow(2.0)
            12\_norm = sum(p.pow(2.0).sum()
                                                                with abs() for L1
                                                                regularization
                          for p in model.parameters())
            loss = loss + 12_lambda * 12_norm
            optimizer.zero_grad()
            loss.backward()
            optimizer.step()
            loss_train += loss.item()
        if epoch == 1 or epoch % 10 == 0:
            print('{} Epoch {}, Training loss {}'.format(
                datetime.datetime.now(), epoch,
                loss_train / len(train_loader)))
```

However, the SGD optimizer in PyTorch already has a weight_decay parameter that corresponds to 2 * lambda, and it directly performs weight decay during the update as described previously. It is fully equivalent to adding the L2 norm of weights to the loss, without the need for accumulating terms in the loss and involving autograd.

NOT RELYING TOO MUCH ON A SINGLE INPUT: DROPOUT

An effective strategy for combating overfitting was originally proposed in 2014 by Nitish Srivastava and coauthors from Geoff Hinton's group in Toronto, in a paper aptly entitled "Dropout: a Simple Way to Prevent Neural Networks from Overfitting" (http://mng.bz/nPMa). Sounds like pretty much exactly what we're looking for,



right? The idea behind dropout is indeed simple: zero out a random fraction of outputs from neurons across the network, where the randomization happens at each training iteration.

This procedure effectively generates slightly different models with different neuron topologies at each iteration, giving neurons in the model less chance to coordinate in the memorization process that happens during overfitting. An alternative point of view is that dropout perturbs the features being generated by the model, exerting an effect that is close to augmentation, but this time throughout the network.

In PyTorch, we can implement dropout in a model by adding an nn.Dropout module between the nonlinear activation function and the linear or convolutional module of the subsequent layer. As an argument, we need to specify the probability with which inputs will be zeroed out. In case of convolutions, we'll use the specialized nn.Dropout2d or nn.Dropout3d, which zero out entire channels of the input:

```
# In[47]:
class NetDropout(nn.Module):
   def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv1_dropout = nn.Dropout2d(p=0.4)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.conv2_dropout = nn.Dropout2d(p=0.4)
        self.fc1 = nn.Linear(8 * 8 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)
   def forward(self, x):
        out = F.max_pool2d(torch.tanh(self.conv1(x)), 2)
        out = self.conv1_dropout(out)
        out = F.max_pool2d(torch.tanh(self.conv2(out)), 2)
        out = self.conv2_dropout(out)
        out = out.view(-1, 8 * 8 * self.n_chans1 // 2)
        out = torch.tanh(self.fc1(out))
        out = self.fc2(out)
        return out
```

Note that dropout is normally active during training, while during the evaluation of a trained model in production, dropout is bypassed or, equivalently, assigned a probability equal to zero. This is controlled through the train property of the Dropout module. Recall that PyTorch lets us switch between the two modalities by calling

```
model.train()
or
model.eval()
```

on any nn.Model subclass. The call will be automatically replicated on the submodules so that if Dropout is among them, it will behave accordingly in subsequent forward and backward passes.

KEEPING ACTIVATIONS IN CHECK: BATCH NORMALIZATION

Dropout was all the rage when, in 2015, another seminal paper was published by Sergey Ioffe and Christian Szegedy from Google, entitled "Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift" (https://arxiv.org/abs/1502.03167). The paper described a technique that had multiple beneficial effects on training: allowing us to increase the learning rate and make training less dependent on initialization and act as a regularizer, thus representing an alternative to dropout.

The main idea behind batch normalization is to rescale the inputs to the activations of the network so that minibatches have a certain desirable distribution. Recalling the mechanics of learning and the role of nonlinear activation functions, this helps avoid the inputs to activation functions being too far into the saturated portion of the function, thereby killing gradients and slowing training.

In practical terms, batch normalization shifts and scales an intermediate input using the mean and standard deviation collected at that intermediate location over the samples of the minibatch. The regularization effect is a result of the fact that an individual sample and its downstream activations are always seen by the model as shifted and scaled, depending on the statistics across the randomly extracted minibatch. This is in itself a form of *principled* augmentation. The authors of the paper suggest that using batch normalization eliminates or at least alleviates the need for dropout.

Batch normalization in PyTorch is provided through the nn.BatchNorm1D, nn.BatchNorm2d, and nn.BatchNorm3d modules, depending on the dimensionality of the input. Since the aim for batch normalization is to rescale the inputs of the activations, the natural location is after the linear transformation (convolution, in this case) and the activation, as shown here:



```
out = self.conv2_batchnorm(self.conv2(out))
out = F.max_pool2d(torch.tanh(out), 2)
out = out.view(-1, 8 * 8 * self.n_chans1 // 2)
out = torch.tanh(self.fc1(out))
out = self.fc2(out)
return out
```

Just as for dropout, batch normalization needs to behave differently during training and inference. In fact, at inference time, we want to avoid having the output for a specific input depend on the statistics of the other inputs we're presenting to the model. As such, we need a way to still normalize, but this time fixing the normalization parameters once and for all.

As numbatches are processed, in addition to estimating the mean and standard deviation for the current minibatch, PyTorch also updates the running estimates for mean and standard deviation that are representative of the whole dataset, as an approximation. This way, when the user specifies

```
model.eval()
```

and the model contains a batch normalization module, the running estimates are frozen and used for normalization. To unfreeze running estimates and return to using the minibatch statistics, we call model.train(), just as we did for dropout.

8.5.3 Going deeper to learn more complex structures: Depth

Earlier, we talked about width as the first dimension to act on in order to make a model larger and, in a way, more capable. The second fundamental dimension is obviously *depth*. Since this is a deep learning book, depth is something we're supposedly into. After all, deeper models are always better than shallow ones, aren't they? Well, it depends. With depth, the complexity of the function the network is able to approximate generally increases. In regard to computer vision, a shallower network could identify a person's shape in a photo, whereas a deeper network could identify the person, the face on their top half, and the mouth within the face. Depth allows a model to deal with hierarchical information when we need to understand the context in order to say something about some input.

There's another way to think about depth: increasing depth is related to increasing the length of the sequence of operations that the network will be able to perform when processing input. This view—of a deep network that performs sequential operations to carry out a task—is likely fascinating to software developers who are used to thinking about algorithms as sequences of operations like "find the person's boundaries, look for the head on top of the boundaries, look for the mouth within the head."

SKIP CONNECTIONS

Depth comes with some additional challenges, which prevented deep learning models from reaching 20 or more layers until late 2015. Adding depth to a model generally makes training harder to converge. Let's recall backpropagation and think about it in

the context of a very deep network. The derivatives of the loss function with respect to the parameters, especially those in early layers, need to be multiplied by a lot of other numbers originating from the chain of derivative operations between the loss and the parameter. Those numbers being multiplied could be small, generating ever-smaller numbers, or large, swallowing smaller numbers due to floating-point approximation. The bottom line is that a long chain of multiplications will tend to make the contribution of the parameter to the gradient *vanish*, leading to ineffective training of that layer since that parameter and others like it won't be properly updated.

In December 2015, Kaiming He and coauthors presented residual networks (ResNets), an architecture that uses a simple trick to allow very deep networks to be successfully trained (https:// arxiv.org/abs/1512.03385). That work opened the door to networks ranging from tens of layers to 100 layers in depth, surpassing the then state of the art in computer vision benchmark problems. We encountered residual networks when we were playing with pretrained models in chapter 2. The trick we mentioned is the following: using a skip connection to short-circuit blocks of layers, as shown in figure 8.11.

A skip connection is nothing but the addition of the input to the output of a block of layers. This is exactly how it is done in PyTorch. Let's add one layer to our simple convolutional model, and let's use ReLU as the activation for a change. The vanilla module with an extra layer looks like this:

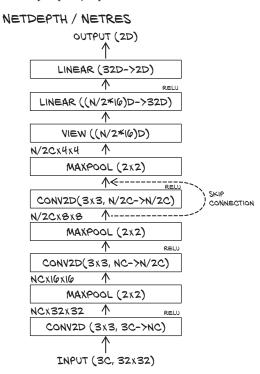


Figure 8.11 The architecture of our network with three convolutional layers. The skip connection is what differentiates NetRes from NetDepth.

```
# In[51]:
class NetDepth(nn.Module):
    def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3, padding=1)
        self.conv3 = nn.Conv2d(n_chans1 // 2, n_chans1 // 2, kernel_size=3, padding=1)
        self.fc1 = nn.Linear(4 * 4 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)
```

```
def forward(self, x):
    out = F.max_pool2d(torch.relu(self.conv1(x)), 2)
    out = F.max_pool2d(torch.relu(self.conv2(out)), 2)
    out = F.max_pool2d(torch.relu(self.conv3(out)), 2)
    out = out.view(-1, 4 * 4 * self.n_chans1 // 2)
    out = torch.relu(self.fc1(out))
    out = self.fc2(out)
    return out
```

Adding a skip connection a la ResNet to this model amounts to adding the output of the first layer in the forward function to the input of the third layer:

```
# In[53]:
class NetRes(nn.Module):
   def __init__(self, n_chans1=32):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.conv2 = nn.Conv2d(n_chans1, n_chans1 // 2, kernel_size=3,
                               padding=1)
        self.conv3 = nn.Conv2d(n_chans1 // 2, n_chans1 // 2,
                               kernel_size=3, padding=1)
        self.fc1 = nn.Linear(4 * 4 * n_chans1 // 2, 32)
        self.fc2 = nn.Linear(32, 2)
   def forward(self, x):
        out = F.max_pool2d(torch.relu(self.conv1(x)), 2)
        out = F.max_pool2d(torch.relu(self.conv2(out)), 2)
        out1 = out
        out = F.max_pool2d(torch.relu(self.conv3(out)) + out1, 2)
        out = out.view(-1, 4 * 4 * self.n_chans1 // 2)
        out = torch.relu(self.fc1(out))
        out = self.fc2(out)
        return out
```

In other words, we're using the output of the first activations as inputs to the last, in addition to the standard feed-forward path. This is also referred to as *identity mapping*. So, how does this alleviate the issues with vanishing gradients we were mentioning earlier?

Thinking about backpropagation, we can appreciate that a skip connection, or a sequence of skip connections in a deep network, creates a direct path from the deeper parameters to the loss. This makes their contribution to the gradient of the loss more direct, as partial derivatives of the loss with respect to those parameters have a chance not to be multiplied by a long chain of other operations.

It has been observed that skip connections have a beneficial effect on convergence especially in the initial phases of training. Also, the loss landscape of deep residual networks is a lot smoother than feed-forward networks of the same depth and width.

It is worth noting that skip connections were not new to the world when ResNets came along. Highway networks and U-Net made use of skip connections of one form

or another. However, the way ResNets used skip connections enabled models of depths greater than 100 to be amenable to training.

Since the advent of ResNets, other architectures have taken skip connections to the next level. One in particular, DenseNet, proposed to connect each layer with several other layers downstream through skip connections, achieving state-of-the-art results with fewer parameters. By now, we know how to implement something like DenseNets: just arithmetically add earlier intermediate outputs to downstream intermediate outputs.

BUILDING VERY DEEP MODELS IN PYTORCH

We talked about exceeding 100 layers in a convolutional neural network. How can we build that network in PyTorch without losing our minds in the process? The standard strategy is to define a building block, such as a (Conv2d, ReLU, Conv2d) + skip connection block, and then build the network dynamically in a for loop. Let's see it done in practice. We will create the network depicted in figure 8.12.

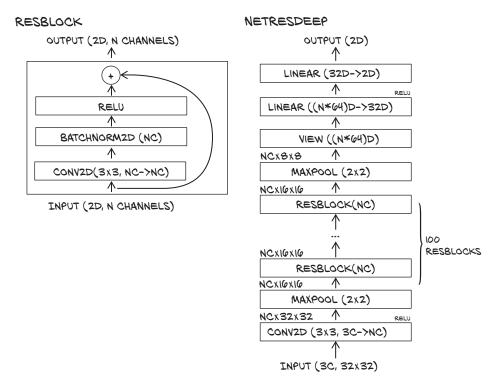


Figure 8.12 Our deep architecture with residual connections. On the left, we define a simplistic residual block. We use it as a building block in our network, as shown on the right.

We first create a module subclass whose sole job is to provide the computation for one *block*—that is, one group of convolutions, activation, and skip connection:

```
# In[55]:
                                                            The BatchNorm layer would
class ResBlock(nn.Module):
                                                             cancel the effect of bias, so
    def __init__(self, n_chans):
                                                               it is customarily left out.
         super(ResBlock, self).__init__()
         self.conv = nn.Conv2d(n_chans, n_chans, kernel_size=3,
                                 padding=1, bias=False)
         self.batch_norm = nn.BatchNorm2d(num_features=n_chans)
         torch.nn.init.kaiming normal (self.conv.weight,
                                           nonlinearity='relu')
         torch.nn.init.constant_(self.batch_norm.weight, 0.5)
         torch.nn.init.zeros_(self.batch_norm.bias)
                                                                  Uses custom initializations
                                                            . kaiming normal initializes with
    def forward(self, x):
         out = self.conv(x)
                                                       normal random elements with standard
                                                    deviation as computed in the ResNet paper.
         out = self.batch_norm(out)
                                                The batch norm is initialized to produce output
         out = torch.relu(out)
                                         distributions that initially have 0 mean and 0.5 variance.
         return out + x
```

Since we're planning to generate a deep model, we are including batch normalization in the block, since this will help prevent gradients from vanishing during training. We'd now like to generate a 100-block network. Does this mean we have to prepare for some serious cutting and pasting? Not at all; we already have the ingredients for imagining how this could look like.

First, in *init*, we create nn.Sequential containing a list of ResBlock instances. nn.Sequential will ensure that the output of one block is used as input to the next. It will also ensure that all the parameters in the block are visible to Net. Then, in forward, we just call the sequential to traverse the 100 blocks and generate the output:

```
# In[56]:
class NetResDeep(nn.Module):
    def __init__(self, n_chans1=32, n_blocks=10):
        super().__init__()
        self.n_chans1 = n_chans1
        self.conv1 = nn.Conv2d(3, n_chans1, kernel_size=3, padding=1)
        self.resblocks = nn.Sequential(
            *(n_blocks * [ResBlock(n_chans=n_chans1)]))
        self.fc1 = nn.Linear(8 * 8 * n_chans1, 32)
        self.fc2 = nn.Linear(32, 2)
    def forward(self, x):
        out = F.max_pool2d(torch.relu(self.conv1(x)), 2)
        out = self.resblocks(out)
        out = F.max_pool2d(out, 2)
        out = out.view(-1, 8 * 8 * self.n_chans1)
        out = torch.relu(self.fc1(out))
        out = self.fc2(out)
        return out
```

In the implementation, we parameterize the actual number of layers, which is important for experimentation and reuse. Also, needless to say, backpropagation will work as expected. Unsurprisingly, the network is quite a bit slower to converge. It is also more

fragile in convergence. This is why we used more-detailed initializations and trained our NetRes with a learning rate of 3e-3 instead of the 1e-2 we used for the other networks. We trained none of the networks to convergence, but we would not have gotten anywhere without these tweaks.

All this shouldn't encourage us to seek depth on a dataset of 32 × 32 images, but it clearly demonstrates how this can be achieved on more challenging datasets like ImageNet. It also provides the key elements for understanding existing implementations for models like ResNet, for instance, in torchvision.

INITIALIZATION

Let's briefly comment about the earlier initialization. Initialization is one of the important tricks in training neural networks. Unfortunately, for historical reasons, PyTorch has default weight initializations that are not ideal. People are looking at fixing the situation; if progress is made, it can be tracked on GitHub (https://github.com/pytorch/pytorch/issues/18182). In the meantime, we need to fix the weight initialization ourselves. We found that our model did not converge and looked at what people commonly choose as initialization (a smaller variance in weights; and zero mean and unit variance outputs for batch norm), and then we had ved the output variance in the batch norm when the network would not converge.

Weight initialization could fill an entire chapter on its own, but we think that would be excessive. In chapter 11, we'll bump into initialization again and use what arguably could be PyTorch defaults without much explanation. Once you've progressed to the point where the details of weight initialization are of specific interest to you—probably not before finishing this book—you might revisit this topic. ¹⁰

8.5.4 Comparing the designs from this section

We summarize the effect of each of our design modifications in isolation in figure 8.13. We should not overinterpret any of the specific numbers—our problem setup and experiments are simplistic, and repeating the experiment with different random seeds will probably generate variation at least as large as the differences in validation accuracy. For this demonstration, we left all other things equal, from learning rate to number of epochs to train; in practice, we would try to get the best results by varying those. Also, we would likely want to combine some of the additional design elements.

But a qualitative observation may be in order: as we saw in section 5.5.3, when discussing validation and overfitting, The weight decay and dropout regularizations, which have a more rigorous statistical estimation interpretation as regularization than batch norm, have a much narrower gap between the two accuracies. Batch norm, which

The seminal paper on the topic is by X. Glorot and Y. Bengio: "Understanding the Difficulty of Training Deep Feedforward Neural Networks" (2010), which introduces PyTorch's *Xavier* initializations (http://mng.bz/vxz7). The ResNet paper we mentioned expands on the topic, too, giving us the Kaiming initializations used earlier. More recently, H. Zhang et al. have tweaked initialization to the point that they do not need batch norm in their experiments with very deep residual networks (https://arxiv.org/abs/1901.09321).

Conclusion 229

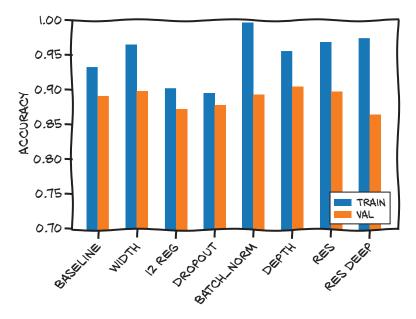


Figure 8.13 The modified networks all perform similarly.

serves more as a convergence helper, lets us train the network to nearly 100% training accuracy, so we interpret the first two as regularization.

8.5.5 It's already outdated

The curse and blessing of a deep learning practitioner is that neural network architectures evolve at a very rapid pace. This is not to say that what we've seen in this chapter is necessarily old school, but a thorough illustration of the latest and greatest architectures is a matter for another book (and they would cease to be the latest and the greatest pretty quickly anyway). The take-home message is that we should make every effort to proficiently translate the math behind a paper into actual PyTorch code, or at least understand the code that others have written with the same intention. In the last few chapters, you have hopefully gathered quite a few of the fundamental skills to translate ideas into implemented models in PyTorch.

8.6 Conclusion

After quite a lot of work, we now have a model that our fictional friend Jane can use to filter images for her blog. All we have to do is take an incoming image, crop and resize it to 32×32 , and see what the model has to say about it. Admittedly, we have solved only part of the problem, but it was a journey in itself.

We have solved just part of the problem because there are a few interesting unknowns we would still have to face. One is picking out a bird or airplane from a larger image. Creating bounding boxes around objects in an image is something a model like ours can't do.

Another hurdle concerns what happens when Fred the cat walks in front of the camera. Our model will not refrain from giving its opinion about how bird-like the cat is! It will happily output "airplane" or "bird," perhaps with 0.99 probability. This issue of being very confident about samples that are far from the training distribution is called *overgeneralization*. It's one of the main problems when we take a (presumably good) model to production in those cases where we can't really trust the input (which, sadly, is the majority of real-world cases).

In this chapter, we have built reasonable, working models in PyTorch that can learn from images. We did it in a way that helped us build our intuition around convolutional networks. We also explored ways in which we can make our models wider and deeper, while controlling effects like overfitting. Although we still only scratched the surface, we have taken another significant step ahead from the previous chapter. We now have a solid basis for facing the challenges we'll encounter when working on deep learning projects.

Now that we're familiar with PyTorch conventions and common features, we're ready to tackle something bigger. We're going to transition from a mode where each chapter or two presents a small problem, to spending multiple chapters breaking down a bigger, real-world problem. Part 2 uses automatic detection of lung cancer as an ongoing example; we will go from being familiar with the PyTorch API to being able to implement entire projects using PyTorch. We'll start in the next chapter by explaining the problem from a high level, and then we'll get into the details of the data we'll be using.

8.7 Exercises

- 1 Change our model to use a 5×5 kernel with kernel_size=5 passed to the nn.Conv2d constructor.
 - a What impact does this change have on the number of parameters in the model?
 - **b** Does the change improve or degrade overfitting?
 - c Read https://pytorch.org/docs/stable/nn.html#conv2d.
 - d Can you describe what kernel_size=(1,3) will do?
 - e How does the model behave with such a kernel?
- 2 Can you find an image that contains neither a bird nor an airplane, but that the model claims has one or the other with more than 95% confidence?
 - a Can you manually edit a neutral image to make it more airplane-like?
 - b Can you manually edit an airplane image to trick the model into reporting a bird?
 - c Do these tasks get easier with a network with less capacity? More capacity?

Summary 231

8.8 **Summary**

 Convolution can be used as the linear operation of a feed-forward network dealing with images. Using convolution produces networks with fewer parameters, exploiting locality and featuring translation invariance.

- Stacking multiple convolutions with their activations one after the other, and using max pooling in between, has the effect of applying convolutions to increasingly smaller feature images, thereby effectively accounting for spatial relationships across larger portions of the input image as depth increases.
- Any nn.Module subclass can recursively collect and return its and its children's parameters. This technique can be used to count them, feed them into the optimizer, or inspect their values.
- The functional API provides modules that do not depend on storing internal state. It is used for operations that do not hold parameters and, hence, are not trained.
- Once trained, parameters of a model can be saved to disk and loaded back in with one line of code each.