MODULE 3

Convolutional Networks

Convolutional networks (LeCun, 1989), also known as convolutional neural networks, or CNNs, are a specialized kind of neural network for processing data that has a known grid-like topology. Examples include time-series data, which can be thought of as a 1-D grid taking samples at regular time intervals, and image data, which can be thought of as a 2-D grid of pixels. Convolutional networks have been tremendously successful in practical applications. The name "convolutional neural network" indicates that the network employs a mathematical operation called convolution. Convolution is a specialized kind of linear operation. Convolutional networks are simply neural networks that use convolution in place of general matrix multiplication in at least one of their layers.

In this chapter, we first describe what convolution is. Next, we explain the motivation behind using convolution in a neural network. We then describe an operation called **pooling**, which almost all convolutional networks employ. Usually, the operation used in a convolutional neural network does not correspond precisely to the definition of convolution as used in other fields, such as engineering or pure mathematics. We describe several variants on the convolution function that are widely used in practice for neural networks. We also show how convolution may be applied to many kinds of data, with different numbers of dimensions. We then discuss means of making convolution more efficient. Convolutional networks stand out as an example of neuroscientific principles influencing deep learning. We discuss these neuroscientific principles, then conclude with comments about the role convolutional networks have played in the history of deep learning. One topic this chapter does not address is how to choose the architecture of your convolutional network. The goal of this chapter is to describe the kinds of tools that convolutional networks provide, while chapter 11 describes general guidelines

for choosing which tools to use in which circumstances. Research into convolutional network architectures proceeds so rapidly that a new best architecture for a given benchmark is announced every few weeks to months, rendering it impractical to describe in print the best architecture. Nonetheless, the best architectures have consistently been composed of the building blocks described here.

9.1 The Convolution Operation

In its most general form, convolution is an operation on two functions of a realvalued argument. To motivate the definition of convolution, we start with examples of two functions we might use.

Suppose we are tracking the location of a spaceship with a laser sensor. Our laser sensor provides a single output x(t), the position of the spaceship at time t. Both x and t are real valued, that is, we can get a different reading from the laser sensor at any instant in time.

Now suppose that our laser sensor is somewhat noisy. To obtain a less noisy estimate of the spaceship's position, we would like to average several measurements. Of course, more recent measurements are more relevant, so we will want this to be a weighted average that gives more weight to recent measurements. We can do this with a weighting function w(a), where a is the age of a measurement. If we apply such a weighted average operation at every moment, we obtain a new function s providing a smoothed estimate of the position of the spaceship:

$$s(t) = \int x(a)w(t-a)da. \tag{9.1}$$

This operation is called **convolution**. The convolution operation is typically denoted with an asterisk:

$$s(t) = (x * w)(t). (9.2)$$

In our example, w needs to be a valid probability density function, or the output will not be a weighted average. Also, w needs to be 0 for all negative arguments, or it will look into the future, which is presumably beyond our capabilities. These limitations are particular to our example, though. In general, convolution is defined for any functions for which the above integral is defined and may be used for other purposes besides taking weighted averages.

In convolutional network terminology, the first argument (in this example, the function x) to the convolution is often referred to as the **input**, and the second

argument (in this example, the function w) as the **kernel**. The output is sometimes referred to as the **feature map**.

In our example, the idea of a laser sensor that can provide measurements at every instant is not realistic. Usually, when we work with data on a computer, time will be discretized, and our sensor will provide data at regular intervals. In our example, it might be more realistic to assume that our laser provides a measurement once per second. The time index t can then take on only integer values. If we now assume that x and w are defined only on integer t, we can define the discrete convolution:

$$s(t) = (x * w)(t) = \sum_{a = -\infty}^{\infty} x(a)w(t - a).$$
 (9.3)

In machine learning applications, the input is usually a multidimensional array of data, and the kernel is usually a multidimensional array of parameters that are adapted by the learning algorithm. We will refer to these multidimensional arrays as tensors. Because each element of the input and kernel must be explicitly stored separately, we usually assume that these functions are zero everywhere but in the finite set of points for which we store the values. This means that in practice, we can implement the infinite summation as a summation over a finite number of array elements.

Finally, we often use convolutions over more than one axis at a time. For example, if we use a two-dimensional image I as our input, we probably also want to use a two-dimensional kernel K:

$$S(i,j) = (I * K)(i,j) = \sum_{m} \sum_{n} I(m,n)K(i-m,j-n).$$
 (9.4)

Convolution is commutative, meaning we can equivalently write

$$S(i,j) = (K*I)(i,j) = \sum_{m} \sum_{n} I(i-m,j-n)K(m,n).$$
 (9.5)

Usually the latter formula is more straightforward to implement in a machine learning library, because there is less variation in the range of valid values of m and n.

The commutative property of convolution arises because we have **flipped** the kernel relative to the input, in the sense that as m increases, the index into the input increases, but the index into the kernel decreases. The only reason to flip the kernel is to obtain the commutative property. While the commutative property

is useful for writing proofs, it is not usually an important property of a neural network implementation. Instead, many neural network libraries implement a related function called the **cross-correlation**, which is the same as convolution but without flipping the kernel:

$$S(i,j) = (K*I)(i,j) = \sum_{m} \sum_{n} I(i+m,j+n)K(m,n).$$
 (9.6)

Many machine learning libraries implement cross-correlation but call it convolution. In this text we follow this convention of calling both operations convolution and specify whether we mean to flip the kernel or not in contexts where kernel flipping is relevant. In the context of machine learning, the learning algorithm will learn the appropriate values of the kernel in the appropriate place, so an algorithm based on convolution with kernel flipping will learn a kernel that is flipped relative to the kernel learned by an algorithm without the flipping. It is also rare for convolution to be used alone in machine learning; instead convolution is used simultaneously with other functions, and the combination of these functions does not commute regardless of whether the convolution operation flips its kernel or not.

See figure 9.1 for an example of convolution (without kernel flipping) applied to a 2-D tensor.

Discrete convolution can be viewed as multiplication by a matrix, but the matrix has several entries constrained to be equal to other entries. For example, for univariate discrete convolution, each row of the matrix is constrained to be equal to the row above shifted by one element. This is known as a **Toeplitz matrix**. In two dimensions, a **doubly block circulant matrix** corresponds to convolution. In addition to these constraints that several elements be equal to each other, convolution usually corresponds to a very sparse matrix (a matrix whose entries are mostly equal to zero). This is because the kernel is usually much smaller than the input image. Any neural network algorithm that works with matrix multiplication and does not depend on specific properties of the matrix structure should work with convolution, without requiring any further changes to the neural network. Typical convolutional neural networks do make use of further specializations in order to deal with large inputs efficiently, but these are not strictly necessary from a theoretical perspective.

9.2 Motivation

Convolution leverages three important ideas that can help improve a machine learning system: sparse interactions, parameter sharing and equivariant

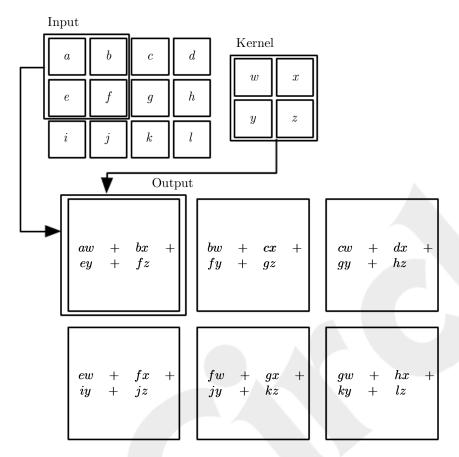


Figure 9.1: An example of 2-D convolution without kernel flipping. We restrict the output to only positions where the kernel lies entirely within the image, called "valid" convolution in some contexts. We draw boxes with arrows to indicate how the upper-left element of the output tensor is formed by applying the kernel to the corresponding upper-left region of the input tensor.

representations. Moreover, convolution provides a means for working with inputs of variable size. We now describe each of these ideas in turn.

Traditional neural network layers use matrix multiplication by a matrix of parameters with a separate parameter describing the interaction between each input unit and each output unit. This means that every output unit interacts with every input unit. Convolutional networks, however, typically have **sparse** interactions (also referred to as **sparse connectivity** or **sparse weights**). This is accomplished by making the kernel smaller than the input. For example, when processing an image, the input image might have thousands or millions of pixels, but we can detect small, meaningful features such as edges with kernels that occupy only tens or hundreds of pixels. This means that we need to store fewer parameters, which both reduces the memory requirements of the model and improves its statistical efficiency. It also means that computing the output

requires fewer operations. These improvements in efficiency are usually quite large. If there are m inputs and n outputs, then matrix multiplication requires $m \times n$ parameters, and the algorithms used in practice have $O(m \times n)$ runtime (per example). If we limit the number of connections each output may have to k, then the sparsely connected approach requires only $k \times n$ parameters and $O(k \times n)$ runtime. For many practical applications, it is possible to obtain good performance on the machine learning task while keeping k several orders of magnitude smaller than m. For graphical demonstrations of sparse connectivity, see figure 9.2 and figure 9.3. In a deep convolutional network, units in the deeper layers may indirectly interact with a larger portion of the input, as shown in figure 9.4. This allows the network to efficiently describe complicated interactions between many variables by constructing such interactions from simple building blocks that each describe only sparse interactions.

Parameter sharing refers to using the same parameter for more than one function in a model. In a traditional neural net, each element of the weight matrix

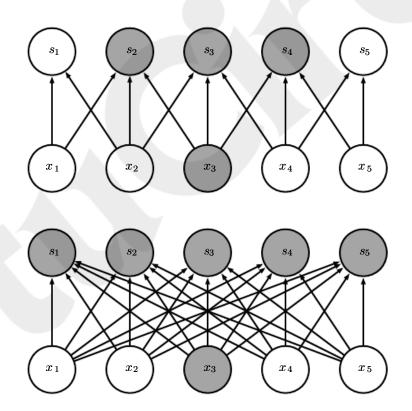


Figure 9.2: Sparse connectivity, viewed from below. We highlight one input unit, x_3 , and highlight the output units in s that are affected by this unit. (Top)When s is formed by convolution with a kernel of width 3, only three outputs are affected by x. (Bottom)When s is formed by matrix multiplication, connectivity is no longer sparse, so all the outputs are affected by x_3 .

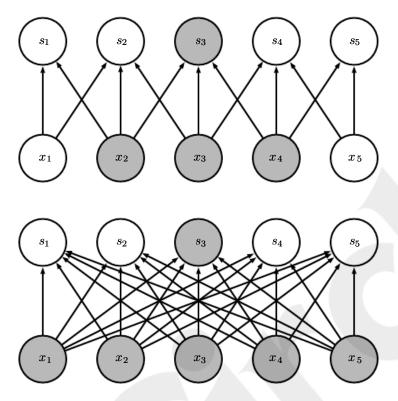


Figure 9.3: Sparse connectivity, viewed from above. We highlight one output unit, s_3 , and highlight the input units in \boldsymbol{x} that affect this unit. These units are known as the **receptive** field of s_3 . (Top)When \boldsymbol{s} is formed by convolution with a kernel of width 3, only three inputs affect s_3 . (Bottom)When \boldsymbol{s} is formed by matrix multiplication, connectivity is no longer sparse, so all the inputs affect s_3 .

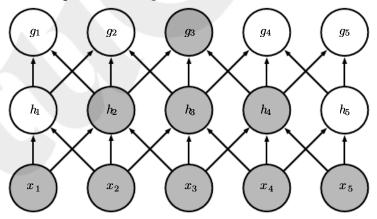


Figure 9.4: The receptive field of the units in the deeper layers of a convolutional network is larger than the receptive field of the units in the shallow layers. This effect increases if the network includes architectural features like strided convolution (figure 9.12) or pooling (section 9.3). This means that even though *direct* connections in a convolutional net are very sparse, units in the deeper layers can be *indirectly* connected to all or most of the input image.

is used exactly once when computing the output of a layer. It is multiplied by one element of the input and then never revisited. As a synonym for parameter sharing, one can say that a network has tied weights, because the value of the weight applied to one input is tied to the value of a weight applied elsewhere. In a convolutional neural net, each member of the kernel is used at every position of the input (except perhaps some of the boundary pixels, depending on the design decisions regarding the boundary). The parameter sharing used by the convolution operation means that rather than learning a separate set of parameters for every location, we learn only one set. This does not affect the runtime of forward propagation—it is still $O(k \times n)$ —but it does further reduce the storage requirements of the model to k parameters. Recall that k is usually several orders of magnitude smaller than m. Since m and n are usually roughly the same size, k is practically insignificant compared to $m \times n$. Convolution is thus dramatically more efficient than dense matrix multiplication in terms of the memory requirements and statistical efficiency. For a graphical depiction of how parameter sharing works, see figure 9.5.

As an example of both of these first two principles in action, figure 9.6 shows how sparse connectivity and parameter sharing can dramatically improve the

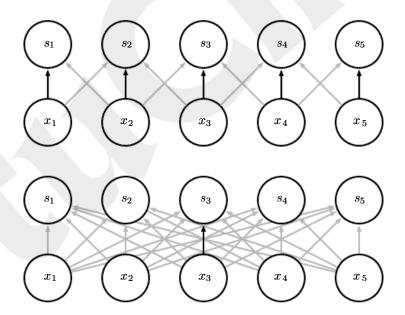


Figure 9.5: Parameter sharing. Black arrows indicate the connections that use a particular parameter in two different models. (Top)The black arrows indicate uses of the central element of a 3-element kernel in a convolutional model. Because of parameter sharing, this single parameter is used at all input locations. (Bottom)The single black arrow indicates the use of the central element of the weight matrix in a fully connected model. This model has no parameter sharing, so the parameter is used only once.



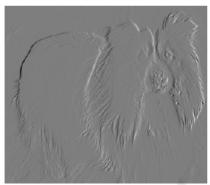


Figure 9.6: Efficiency of edge detection. The image on the right was formed by taking each pixel in the original image and subtracting the value of its neighboring pixel on the left. This shows the strength of all the vertically oriented edges in the input image, which can be a useful operation for object detection. Both images are 280 pixels tall. The input image is 320 pixels wide, while the output image is 319 pixels wide. This transformation can be described by a convolution kernel containing two elements, and requires $319 \times 280 \times 3 = 267,960$ floating-point operations (two multiplications and one addition per output pixel) to compute using convolution. To describe the same transformation with a matrix multiplication would take $320 \times 280 \times 319 \times 280$, or over eight billion, entries in the matrix, making convolution four billion times more efficient for representing this transformation. The straightforward matrix multiplication algorithm performs over sixteen billion floating point operations, making convolution roughly 60,000 times more efficient computationally. Of course, most of the entries of the matrix would be zero. If we stored only the nonzero entries of the matrix, then both matrix multiplication and convolution would require the same number of floating-point operations to compute. The matrix would still need to contain $2 \times 319 \times 280 = 178,640$ entries. Convolution is an extremely efficient way of describing transformations that apply the same linear transformation of a small local region across the entire input. Photo credit: Paula Goodfellow.

efficiency of a linear function for detecting edges in an image.

In the case of convolution, the particular form of parameter sharing causes the layer to have a property called **equivariance** to translation. To say a function is equivariant means that if the input changes, the output changes in the same way. Specifically, a function f(x) is equivariant to a function g if f(g(x)) = g(f(x)). In the case of convolution, if we let g be any function that translates the input, that is, shifts it, then the convolution function is equivariant to g. For example, let f be a function giving image brightness at integer coordinates. Let f be a function mapping one image function to another image function, such that f' = g(f) is the image function with f'(x,y) = f(x-1,y). This shifts every pixel of f one unit to the right. If we apply this transformation to f, then applied the transformation will be the same as if we applied convolution to f, then applied the transformation

g to the output. When processing time-series data, this means that convolution produces a sort of timeline that shows when different features appear in the input. If we move an event later in time in the input, the exact same representation of it will appear in the output, just later. Similarly with images, convolution creates a 2-D map of where certain features appear in the input. If we move the object in the input, its representation will move the same amount in the output. This is useful for when we know that some function of a small number of neighboring pixels is useful when applied to multiple input locations. For example, when processing images, it is useful to detect edges in the first layer of a convolutional network. The same edges appear more or less everywhere in the image, so it is practical to share parameters across the entire image. In some cases, we may not wish to share parameters across the entire image. For example, if we are processing images that are cropped to be centered on an individual's face, we probably want to extract different features at different locations—the part of the network processing the top of the face needs to look for eyebrows, while the part of the network processing the bottom of the face needs to look for a chin.

Convolution is not naturally equivariant to some other transformations, such as changes in the scale or rotation of an image. Other mechanisms are necessary for handling these kinds of transformations.

Finally, some kinds of data cannot be processed by neural networks defined by matrix multiplication with a fixed-shape matrix. Convolution enables processing of some of these kinds of data. We discuss this further in section 9.7.

9.3 Pooling

A typical layer of a convolutional network consists of three stages (see figure 9.7). In the first stage, the layer performs several convolutions in parallel to produce a set of linear activations. In the second stage, each linear activation is run through a nonlinear activation function, such as the rectified linear activation function. This stage is sometimes called the **detector stage**. In the third stage, we use a **pooling function** to modify the output of the layer further.

A pooling function replaces the output of the net at a certain location with a summary statistic of the nearby outputs. For example, the **max pooling** (Zhou and Chellappa, 1988) operation reports the maximum output within a rectangular neighborhood. Other popular pooling functions include the average of a rectangular neighborhood, the L^2 norm of a rectangular neighborhood, or a weighted average based on the distance from the central pixel.

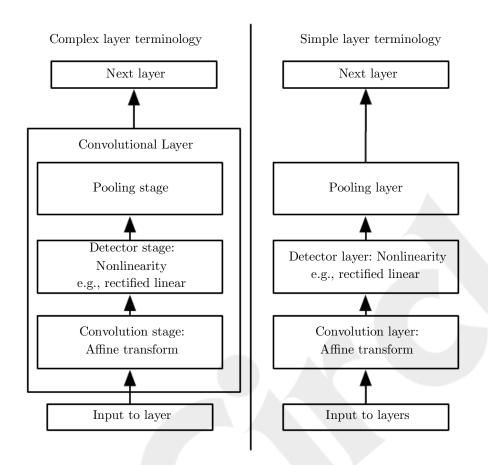


Figure 9.7: The components of a typical convolutional neural network layer. There are two commonly used sets of terminology for describing these layers. (Left)In this terminology, the convolutional net is viewed as a small number of relatively complex layers, with each layer having many "stages." In this terminology, there is a one-to-one mapping between kernel tensors and network layers. In this book we generally use this terminology. (Right)In this terminology, the convolutional net is viewed as a larger number of simple layers; every step of processing is regarded as a layer in its own right. This means that not every "layer" has parameters.

In all cases, pooling helps to make the representation approximately **invariant** to small translations of the input. Invariance to translation means that if we translate the input by a small amount, the values of most of the pooled outputs do not change. See figure 9.8 for an example of how this works. *Invariance to local translation can be a useful property if we care more about whether some feature is present than exactly where it is.* For example, when determining whether an image contains a face, we need not know the location of the eyes with pixel-perfect accuracy, we just need to know that there is an eye on the left side of the face and an eye on the right side of the face. In other contexts, it is more important to preserve the location of a feature. For example, if we want to find a corner defined

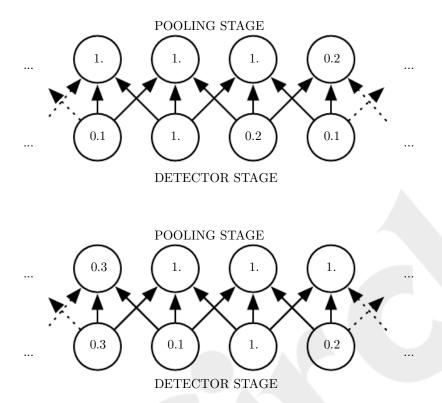


Figure 9.8: Max pooling introduces invariance. (Top)A view of the middle of the output of a convolutional layer. The bottom row shows outputs of the nonlinearity. The top row shows the outputs of max pooling, with a stride of one pixel between pooling regions and a pooling region width of three pixels. (Bottom)A view of the same network, after the input has been shifted to the right by one pixel. Every value in the bottom row has changed, but only half of the values in the top row have changed, because the max pooling units are sensitive only to the maximum value in the neighborhood, not its exact location.

by two edges meeting at a specific orientation, we need to preserve the location of the edges well enough to test whether they meet.

The use of pooling can be viewed as adding an infinitely strong prior that the function the layer learns must be invariant to small translations. When this assumption is correct, it can greatly improve the statistical efficiency of the network.

Pooling over spatial regions produces invariance to translation, but if we pool over the outputs of separately parametrized convolutions, the features can learn which transformations to become invariant to (see figure 9.9).

Because pooling summarizes the responses over a whole neighborhood, it is possible to use fewer pooling units than detector units, by reporting summary statistics for pooling regions spaced k pixels apart rather than 1 pixel apart. See figure 9.10 for an example. This improves the computational efficiency of the network because the next layer has roughly k times fewer inputs to process. When

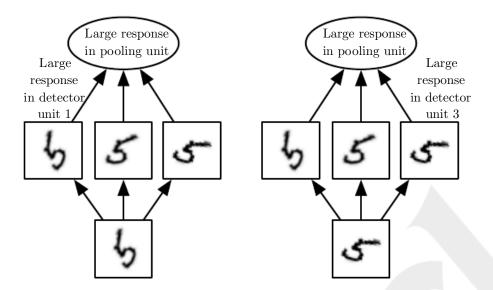


Figure 9.9: Example of learned invariances. A pooling unit that pools over multiple features that are learned with separate parameters can learn to be invariant to transformations of the input. Here we show how a set of three learned filters and a max pooling unit can learn to become invariant to rotation. All three filters are intended to detect a hand written 5. Each filter attempts to match a slightly different orientation of the 5. When a 5 appears in the input, the corresponding filter will match it and cause a large activation in a detector unit. The max pooling unit then has a large activation regardless of which detector unit was activated. We show here how the network processes two different inputs, resulting in two different detector units being activated. The effect on the pooling unit is roughly the same either way. This principle is leveraged by maxout networks (Goodfellow et al., 2013a) and other convolutional networks. Max pooling over spatial positions is naturally invariant to translation; this multichannel approach is only necessary for learning other transformations.

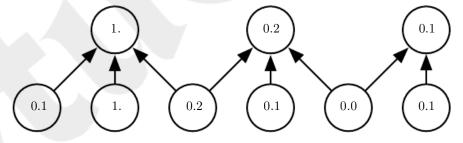


Figure 9.10: Pooling with downsampling. Here we use max pooling with a pool width of three and a stride between pools of two. This reduces the representation size by a factor of two, which reduces the computational and statistical burden on the next layer. Note that the rightmost pooling region has a smaller size but must be included if we do not want to ignore some of the detector units.

the number of parameters in the next layer is a function of its input size (such as when the next layer is fully connected and based on matrix multiplication), this

reduction in the input size can also result in improved statistical efficiency and reduced memory requirements for storing the parameters.

For many tasks, pooling is essential for handling inputs of varying size. For example, if we want to classify images of variable size, the input to the classification layer must have a fixed size. This is usually accomplished by varying the size of an offset between pooling regions so that the classification layer always receives the same number of summary statistics regardless of the input size. For example, the final pooling layer of the network may be defined to output four sets of summary statistics, one for each quadrant of an image, regardless of the image size.

Some theoretical work gives guidance as to which kinds of pooling one should use in various situations (Boureau et al., 2010). It is also possible to dynamically pool features together, for example, by running a clustering algorithm on the locations of interesting features (Boureau et al., 2011). This approach yields a different set of pooling regions for each image. Another approach is to learn a single pooling structure that is then applied to all images (Jia et al., 2012).

Pooling can complicate some kinds of neural network architectures that use top-down information, such as Boltzmann machines and autoencoders. These issues are discussed further when we present these types of networks in part III. Pooling in convolutional Boltzmann machines is presented in section 20.6. The inverse-like operations on pooling units needed in some differentiable networks are covered in section 20.10.6.

Some examples of complete convolutional network architectures for classification using convolution and pooling are shown in figure 9.11.

9.4 Convolution and Pooling as an Infinitely Strong Prior

Recall the concept of a **prior probability distribution** from section 5.6. This is a probability distribution over the parameters of a model that encodes our beliefs about what models are reasonable, before we have seen any data.

Priors can be considered weak or strong depending on how concentrated the probability density in the prior is. A weak prior is a prior distribution with high entropy, such as a Gaussian distribution with high variance. Such a prior allows the data to move the parameters more or less freely. A strong prior has very low entropy, such as a Gaussian distribution with low variance. Such a prior plays a more active role in determining where the parameters end up.

An infinitely strong prior places zero probability on some parameters and says



Figure 9.11: Examples of architectures for classification with convolutional networks. The specific strides and depths used in this figure are not advisable for real use; they are designed to be very shallow to fit onto the page. Real convolutional networks also often involve significant amounts of branching, unlike the chain structures used here for simplicity. (Left)A convolutional network that processes a fixed image size. After alternating between convolution and pooling for a few layers, the tensor for the convolutional feature map is reshaped to flatten out the spatial dimensions. The rest of the network is an ordinary feedforward network classifier, as described in chapter 6. (Center)A convolutional network that processes a variably sized image but still maintains a fully connected section. This network uses a pooling operation with variably sized pools but a fixed number of pools, in order to provide a fixed-size vector of 576 units to the fully connected portion of the network. (Right) A convolutional network that does not have any fully connected weight layer. Instead, the last convolutional layer outputs one feature map per class. The model presumably learns a map of how likely each class is to occur at each spatial location. Averaging a feature map down to a single value provides the argument to the softmax classifier at the top.

that these parameter values are completely forbidden, regardless of how much support the data give to those values.

We can imagine a convolutional net as being similar to a fully connected net, but with an infinitely strong prior over its weights. This infinitely strong prior says that the weights for one hidden unit must be identical to the weights of its neighbor but shifted in space. The prior also says that the weights must be zero, except for in the small, spatially contiguous receptive field assigned to that hidden unit. Overall, we can think of the use of convolution as introducing an infinitely strong prior probability distribution over the parameters of a layer. This prior says that the function the layer should learn contains only local interactions and is equivariant to translation. Likewise, the use of pooling is an infinitely strong prior that each unit should be invariant to small translations.

Of course, implementing a convolutional net as a fully connected net with an infinitely strong prior would be extremely wasteful computationally. But thinking of a convolutional net as a fully connected net with an infinitely strong prior can give us some insights into how convolutional nets work.

One key insight is that convolution and pooling can cause underfitting. Like any prior, convolution and pooling are only useful when the assumptions made by the prior are reasonably accurate. If a task relies on preserving precise spatial information, then using pooling on all features can increase the training error. Some convolutional network architectures (Szegedy et al., 2014a) are designed to use pooling on some channels but not on other channels, in order to get both highly invariant features and features that will not underfit when the translation invariance prior is incorrect. When a task involves incorporating information from very distant locations in the input, then the prior imposed by convolution may be inappropriate.

Another key insight from this view is that we should only compare convolutional models to other convolutional models in benchmarks of statistical learning performance. Models that do not use convolution would be able to learn even if we permuted all the pixels in the image. For many image datasets, there are separate benchmarks for models that are **permutation invariant** and must discover the concept of topology via learning and for models that have the knowledge of spatial relationships hard coded into them by their designer.

9.5 Variants of the Basic Convolution Function

When discussing convolution in the context of neural networks, we usually do not refer exactly to the standard discrete convolution operation as it is usually understood in the mathematical literature. The functions used in practice differ slightly. Here we describe these differences in detail and highlight some useful properties of the functions used in neural networks.

First, when we refer to convolution in the context of neural networks, we usually actually mean an operation that consists of many applications of convolution in parallel. This is because convolution with a single kernel can extract only one kind of feature, albeit at many spatial locations. Usually we want each layer of our network to extract many kinds of features, at many locations.

Additionally, the input is usually not just a grid of real values. Rather, it is a grid of vector-valued observations. For example, a color image has a red, green and blue intensity at each pixel. In a multilayer convolutional network, the input to the second layer is the output of the first layer, which usually has the output of many different convolutions at each position. When working with images, we usually think of the input and output of the convolution as being 3-D tensors, with one index into the different channels and two indices into the spatial coordinates of each channel. Software implementations usually work in batch mode, so they will actually use 4-D tensors, with the fourth axis indexing different examples in the batch, but we will omit the batch axis in our description here for simplicity.

Because convolutional networks usually use multichannel convolution, the linear operations they are based on are not guaranteed to be commutative, even if kernel flipping is used. These multichannel operations are only commutative if each operation has the same number of output channels as input channels.

Assume we have a 4-D kernel tensor K with element $K_{i,j,k,l}$ giving the connection strength between a unit in channel i of the output and a unit in channel j of the input, with an offset of k rows and l columns between the output unit and the input unit. Assume our input consists of observed data V with element $V_{i,j,k}$ giving the value of the input unit within channel i at row j and column k. Assume our output consists of Z with the same format as V. If Z is produced by convolving K across V without flipping K, then

$$Z_{i,j,k} = \sum_{l,m,n} V_{l,j+m-1,k+n-1} K_{i,l,m,n}, \qquad (9.7)$$

where the summation over l, m and n is over all values for which the tensor indexing operations inside the summation are valid. In linear algebra notation,

we index into arrays using a 1 for the first entry. This necessitates the -1 in the above formula. Programming languages such as C and Python index starting from 0, rendering the above expression even simpler.

We may want to skip over some positions of the kernel to reduce the computational cost (at the expense of not extracting our features as finely). We can think of this as downsampling the output of the full convolution function. If we want to sample only every s pixels in each direction in the output, then we can define a downsampled convolution function c such that

$$Z_{i,j,k} = c(\mathbf{K}, \mathbf{V}, s)_{i,j,k} = \sum_{l,m,n} \left[V_{l,(j-1)\times s+m,(k-1)\times s+n} K_{i,l,m,n} \right].$$
 (9.8)

We refer to s as the **stride** of this downsampled convolution. It is also possible to define a separate stride for each direction of motion. See figure 9.12 for an illustration.

One essential feature of any convolutional network implementation is the ability to implicitly zero pad the input **V** to make it wider. Without this feature, the width of the representation shrinks by one pixel less than the kernel width at each layer. Zero padding the input allows us to control the kernel width and the size of the output independently. Without zero padding, we are forced to choose between shrinking the spatial extent of the network rapidly and using small kernels—both scenarios that significantly limit the expressive power of the network. See figure 9.13 for an example.

Three special cases of the zero-padding setting are worth mentioning. One is the extreme case in which no zero padding is used whatsoever, and the convolution kernel is allowed to visit only positions where the entire kernel is contained entirely within the image. In MATLAB terminology, this is called valid convolution. In this case, all pixels in the output are a function of the same number of pixels in the input, so the behavior of an output pixel is somewhat more regular. However, the size of the output shrinks at each layer. If the input image has width m and the kernel has width k, the output will be of width m-k+1. The rate of this shrinkage can be dramatic if the kernels used are large. Since the shrinkage is greater than 0, it limits the number of convolutional layers that can be included in the network. As layers are added, the spatial dimension of the network will eventually drop to 1×1 , at which point additional layers cannot meaningfully be considered convolutional. Another special case of the zero-padding setting is when just enough zero padding is added to keep the size of the output equal to the size of the input. MATLAB calls this **same** convolution. In this case, the network can contain as many convolutional layers as the available hardware can support, since the operation of convolution does not modify the architectural possibilities

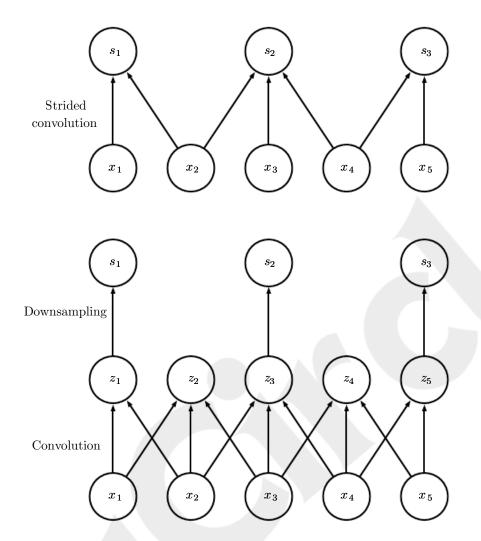


Figure 9.12: Convolution with a stride. In this example, we use a stride of two. (Top)Convolution with a stride length of two implemented in a single operation. (Bottom)Convolution with a stride greater than one pixel is mathematically equivalent to convolution with unit stride followed by downsampling. Obviously, the two-step approach involving downsampling is computationally wasteful, because it computes many values that are then discarded.

available to the next layer. The input pixels near the border, however, influence fewer output pixels than the input pixels near the center. This can make the border pixels somewhat underrepresented in the model. This motivates the other extreme case, which MATLAB refers to as **full** convolution, in which enough zeros are added for every pixel to be visited k times in each direction, resulting in an output image of width m + k - 1. In this case, the output pixels near the border are a function of fewer pixels than the output pixels near the center. This can make it difficult to learn a single kernel that performs well at all positions in the convolutional feature map. Usually the optimal amount of zero padding (in

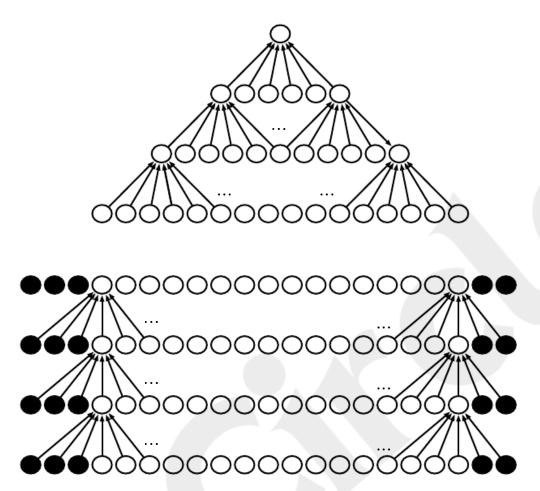


Figure 9.13: The effect of zero padding on network size. Consider a convolutional network with a kernel of width six at every layer. In this example, we do not use any pooling, so only the convolution operation itself shrinks the network size. (Top)In this convolutional network, we do not use any implicit zero padding. This causes the representation to shrink by five pixels at each layer. Starting from an input of sixteen pixels, we are only able to have three convolutional layers, and the last layer does not ever move the kernel, so arguably only two of the layers are truly convolutional. The rate of shrinking can be mitigated by using smaller kernels, but smaller kernels are less expressive, and some shrinking is inevitable in this kind of architecture. (Bottom)By adding five implicit zeros to each layer, we prevent the representation from shrinking with depth. This allows us to make an arbitrarily deep convolutional network.

terms of test set classification accuracy) lies somewhere between "valid" and "same" convolution.

In some cases, we do not actually want to use convolution, but want to use locally connected layers instead (LeCun, 1986, 1989). In this case, the adjacency matrix in the graph of our MLP is the same, but every connection has its own weight, specified by a 6-D tensor **W**. The indices into **W** are respectively: *i*; the

output channel; j, the output row; k, the output column; l, the input channel; m, the row offset within the input; and n, the column offset within the input. The linear part of a locally connected layer is then given by

$$Z_{i,j,k} = \sum_{l,m,n} \left[V_{l,j+m-1,k+n-1} w_{i,j,k,l,m,n} \right]. \tag{9.9}$$

This is sometimes also called **unshared convolution**, because it is a similar operation to discrete convolution with a small kernel, but without sharing parameters across locations. Figure 9.14 compares local connections, convolution, and full connections.

Locally connected layers are useful when we know that each feature should be a function of a small part of space, but there is no reason to think that the same feature should occur across all of space. For example, if we want to tell if an image is a picture of a face, we only need to look for the mouth in the bottom half of the image.

It can also be useful to make versions of convolution or locally connected layers in which the connectivity is further restricted, for example to constrain each output channel i to be a function of only a subset of the input channels l. A common way to do this is to make the first m output channels connect to only the first n input channels, the second m output channels connect to only the second m input channels, and so on. See figure 9.15 for an example. Modeling interactions between few channels allows the network to have fewer parameters, reducing memory consumption, increasing statistical efficiency, and reducing the amount of computation needed to perform forward and back-propagation. It accomplishes these goals without reducing the number of hidden units.

Tiled convolution (Gregor and LeCun, 2010a; Le et al., 2010) offers a compromise between a convolutional layer and a locally connected layer. Rather than learning a separate set of weights at every spatial location, we learn a set of kernels that we rotate through as we move through space. This means that immediately neighboring locations will have different filters, as in a locally connected layer, but the memory requirements for storing the parameters will increase only by a factor of the size of this set of kernels, rather than by the size of the entire output feature map. See figure 9.16 for a comparison of locally connected layers, tiled convolution, and standard convolution.

To define tiled convolution algebraically, let K be a 6-D tensor, where two of the dimensions correspond to different locations in the output map. Rather than having a separate index for each location in the output map, output locations cycle through a set of t different choices of kernel stack in each direction. If t is equal to

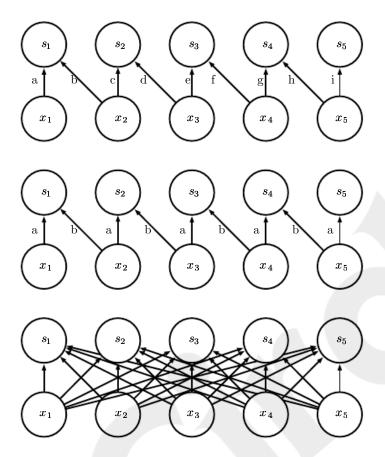


Figure 9.14: Comparison of local connections, convolution, and full connections. (Top)A locally connected layer with a patch size of two pixels. Each edge is labeled with a unique letter to show that each edge is associated with its own weight parameter. (Center)A convolutional layer with a kernel width of two pixels. This model has exactly the same connectivity as the locally connected layer. The difference lies not in which units interact with each other, but in how the parameters are shared. The locally connected layer has no parameter sharing. The convolutional layer uses the same two weights repeatedly across the entire input, as indicated by the repetition of the letters labeling each edge. (Bottom)A fully connected layer resembles a locally connected layer in the sense that each edge has its own parameter (there are too many to label explicitly with letters in this diagram). It does not, however, have the restricted connectivity of the locally connected layer.

the output width, this is the same as a locally connected layer.

$$Z_{i,j,k} = \sum_{l,m,n} V_{l,j+m-1,k+n-1} K_{i,l,m,n,j\%t+1,k\%t+1}, \qquad (9.10)$$

where percent is the modulo operation, with t % t = 0, (t+1)% t = 1, and so on. It is straightforward to generalize this equation to use a different tiling range for each dimension.

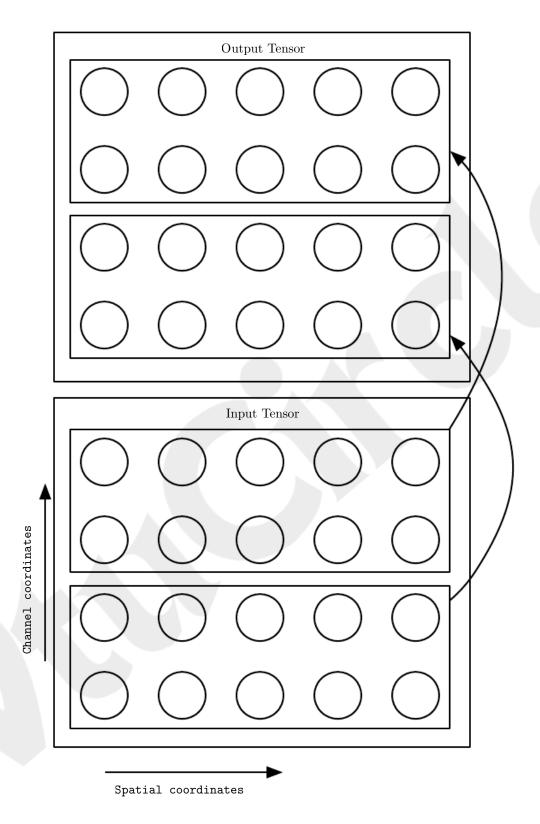


Figure 9.15: A convolutional network with the first two output channels connected to only the first two input channels, and the second two output channels connected to only the second two input channels.

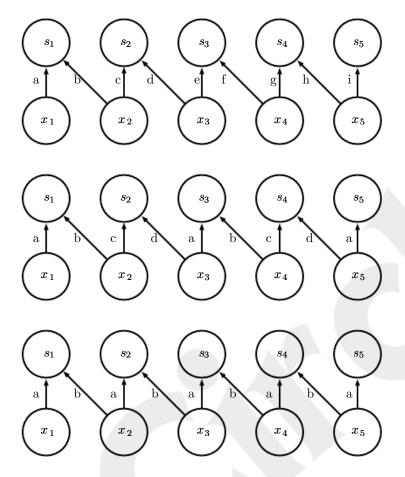


Figure 9.16: A comparison of locally connected layers, tiled convolution, and standard convolution. All three have the same sets of connections between units, when the same size of kernel is used. This diagram illustrates the use of a kernel that is two pixels wide. The differences between the methods lies in how they share parameters. (Top) A locally connected layer has no sharing at all. We indicate that each connection has its own weight by labeling each connection with a unique letter. (Center) Tiled convolution has a set of t different kernels. Here we illustrate the case of t = 2. One of these kernels has edges labeled "a" and "b," while the other has edges labeled "c" and "d." Each time we move one pixel to the right in the output, we move on to using a different kernel. This means that, like the locally connected layer, neighboring units in the output have different parameters. Unlike the locally connected layer, after we have gone through all t available kernels, we cycle back to the first kernel. If two output units are separated by a multiple of t steps, then they share parameters. (Bottom) Traditional convolution is equivalent to tiled convolution with t = 1. There is only one kernel, and it is applied everywhere, as indicated in the diagram by using the kernel with weights labeled "a" and "b" everywhere.

Locally connected layers and tiled convolutional layers both have an interesting interaction with max pooling: the detector units of these layers are driven by different filters. If these filters learn to detect different transformed versions of

the same underlying features, then the max-pooled units become invariant to the learned transformation (see figure 9.9). Convolutional layers are hard coded to be invariant specifically to translation.

Other operations besides convolution are usually necessary to implement a convolutional network. To perform learning, one must be able to compute the gradient with respect to the kernel, given the gradient with respect to the outputs. In some simple cases, this operation can be performed using the convolution operation, but many cases of interest, including the case of stride greater than 1, do not have this property.

Recall that convolution is a linear operation and can thus be described as a matrix multiplication (if we first reshape the input tensor into a flat vector). The matrix involved is a function of the convolution kernel. The matrix is sparse, and each element of the kernel is copied to several elements of the matrix. This view helps us to derive some of the other operations needed to implement a convolutional network.

Multiplication by the transpose of the matrix defined by convolution is one such operation. This is the operation needed to back-propagate error derivatives through a convolutional layer, so it is needed to train convolutional networks that have more than one hidden layer. This same operation is also needed if we wish to reconstruct the visible units from the hidden units (Simard et al., 1992). Reconstructing the visible units is an operation commonly used in the models described in part III of this book, such as autoencoders, RBMs, and sparse coding. Transpose convolution is necessary to construct convolutional versions of those models. Like the kernel gradient operation, this input gradient operation can sometimes be implemented using a convolution but in general requires a third operation to be implemented. Care must be taken to coordinate this transpose operation with the forward propagation. The size of the output that the transpose operation should return depends on the zero-padding policy and stride of the forward propagation operation, as well as the size of the forward propagation's output map. In some cases, multiple sizes of input to forward propagation can result in the same size of output map, so the transpose operation must be explicitly told what the size of the original input was.

These three operations—convolution, backprop from output to weights, and backprop from output to inputs—are sufficient to compute all the gradients needed to train any depth of feedforward convolutional network, as well as to train convolutional networks with reconstruction functions based on the transpose of convolution. See Goodfellow (2010) for a full derivation of the equations in the fully general multidimensional, multiexample case. To give a sense of how these

equations work, we present the two-dimensional, single example version here.

Suppose we want to train a convolutional network that incorporates strided convolution of kernel stack K applied to multichannel image V with stride s as defined by c(K, V, s), as in equation 9.8. Suppose we want to minimize some loss function J(V, K). During forward propagation, we will need to use c itself to output Z, which is then propagated through the rest of the network and used to compute the cost function J. During back-propagation, we will receive a tensor G such that $G_{i,j,k} = \frac{\partial}{\partial Z_{i,j,k}} J(V, K)$.

To train the network, we need to compute the derivatives with respect to the weights in the kernel. To do so, we can use a function

$$g(\mathbf{G}, \mathbf{V}, s)_{i,j,k,l} = \frac{\partial}{\partial \mathcal{K}_{i,j,k,l}} J(\mathbf{V}, \mathbf{K}) = \sum_{m,n} G_{i,m,n} V_{j,(m-1)\times s+k,(n-1)\times s+l}.$$
(9.11)

If this layer is not the bottom layer of the network, we will need to compute the gradient with respect to \boldsymbol{V} to back-propagate the error further down. To do so, we can use a function

$$h(\mathbf{K}, \mathbf{G}, s)_{i,j,k} = \frac{\partial}{\partial V_{i,j,k}} J(\mathbf{V}, \mathbf{K})$$
(9.12)

$$= \sum_{\substack{l,m \\ \text{s.t.} \\ (l-1) \times s+m=j \ (n-1) \times s+p=k}} \sum_{\substack{n,p \\ \text{s.t.} \\ (n-1) \times s+p=k}} \sum_{q} K_{q,i,m,p} G_{q,l,n}.$$
 (9.13)

Autoencoder networks, described in chapter 14, are feedforward networks trained to copy their input to their output. A simple example is the PCA algorithm, which copies its input \boldsymbol{x} to an approximate reconstruction \boldsymbol{r} using the function $\boldsymbol{W}^{\top}\boldsymbol{W}\boldsymbol{x}$. It is common for more general autoencoders to use multiplication by the transpose of the weight matrix just as PCA does. To make such models convolutional, we can use the function h to perform the transpose of the convolution operation. Suppose we have hidden units $\boldsymbol{\mathsf{H}}$ in the same format as $\boldsymbol{\mathsf{Z}}$ and we define a reconstruction

$$\mathbf{R} = h(\mathbf{K}, \mathbf{H}, s). \tag{9.14}$$

To train the autoencoder, we will receive the gradient with respect to \mathbf{R} as a tensor \mathbf{E} . To train the decoder, we need to obtain the gradient with respect to \mathbf{K} . This is given by $g(\mathbf{H}, \mathbf{E}, s)$. To train the encoder, we need to obtain the gradient with respect to \mathbf{H} . This is given by $c(\mathbf{K}, \mathbf{E}, s)$. It is also possible to differentiate through g using c and h, but these operations are not needed for the back-propagation algorithm on any standard network architectures.

Generally, we do not use only a linear operation to transform from the inputs to the outputs in a convolutional layer. We generally also add some bias term to each output before applying the nonlinearity. This raises the question of how to share parameters among the biases. For locally connected layers, it is natural to give each unit its own bias, and for tiled convolution, it is natural to share the biases with the same tiling pattern as the kernels. For convolutional layers, it is typical to have one bias per channel of the output and share it across all locations within each convolution map. If the input is of known, fixed size, however, it is also possible to learn a separate bias at each location of the output map. Separating the biases may slightly reduce the statistical efficiency of the model, but it allows the model to correct for differences in the image statistics at different locations. For example, when using implicit zero padding, detector units at the edge of the image receive less total input and may need larger biases.

9.6 Structured Outputs

Convolutional networks can be used to output a high-dimensional structured object, rather than just predicting a class label for a classification task or a real value for a regression task. Typically this object is just a tensor, emitted by a standard convolutional layer. For example, the model might emit a tensor \mathbf{S} , where $S_{i,j,k}$ is the probability that pixel (j,k) of the input to the network belongs to class i. This allows the model to label every pixel in an image and draw precise masks that follow the outlines of individual objects.

One issue that often comes up is that the output plane can be smaller than the input plane, as shown in figure 9.13. In the kinds of architectures typically used for classification of a single object in an image, the greatest reduction in the spatial dimensions of the network comes from using pooling layers with large stride. To produce an output map of similar size as the input, one can avoid pooling altogether (Jain et al., 2007). Another strategy is to simply emit a lower-resolution grid of labels (Pinheiro and Collobert, 2014, 2015). Finally, in principle, one could use a pooling operator with unit stride.

One strategy for pixel-wise labeling of images is to produce an initial guess of the image labels, then refine this initial guess using the interactions between neighboring pixels. Repeating this refinement step several times corresponds to using the same convolutions at each stage, sharing weights between the last layers of the deep net (Jain et al., 2007). This makes the sequence of computations performed by the successive convolutional layers with weights shared across layers a particular

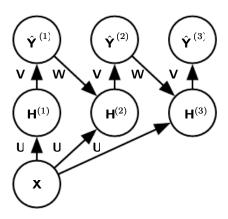


Figure 9.17: An example of a recurrent convolutional network for pixel labeling. The input is an image tensor \mathbf{X} , with axes corresponding to image rows, image columns, and channels (red, green, blue). The goal is to output a tensor of labels \hat{Y} , with a probability distribution over labels for each pixel. This tensor has axes corresponding to image rows, image columns, and the different classes. Rather than outputting \hat{Y} in a single shot, the recurrent network iteratively refines its estimate \hat{Y} by using a previous estimate of \hat{Y} as input for creating a new estimate. The same parameters are used for each updated estimate, and the estimate can be refined as many times as we wish. The tensor of convolution kernels \mathbf{U} is used on each step to compute the hidden representation given the input image. The kernel tensor \mathbf{V} is used to produce an estimate of the labels given the hidden values. On all but the first step, the kernels \mathbf{W} are convolved over \hat{Y} to provide input to the hidden layer. On the first time step, this term is replaced by zero. Because the same parameters are used on each step, this is an example of a recurrent network, as described in chapter $\mathbf{10}$.

kind of recurrent network (Pinheiro and Collobert, 2014, 2015). Figure 9.17 shows the architecture of such a recurrent convolutional network.

Once a prediction for each pixel is made, various methods can be used to further process these predictions to obtain a segmentation of the image into regions (Briggman et al., 2009; Turaga et al., 2010; Farabet et al., 2013). The general idea is to assume that large groups of contiguous pixels tend to be associated with the same label. Graphical models can describe the probabilistic relationships between neighboring pixels. Alternatively, the convolutional network can be trained to maximize an approximation of the graphical model training objective (Ning et al., 2005; Thompson et al., 2014).

9.7 Data Types

The data used with a convolutional network usually consist of several channels, each channel being the observation of a different quantity at some point in space or time. See table 9.1 for examples of data types with different dimensionalities and number of channels.

For an example of convolutional networks applied to video, see Chen *et al.* (2010).

So far we have discussed only the case where every example in the train and test data has the same spatial dimensions. One advantage to convolutional networks is that they can also process inputs with varying spatial extents. These kinds of input simply cannot be represented by traditional, matrix multiplication-based neural networks. This provides a compelling reason to use convolutional networks even when computational cost and overfitting are not significant issues.

For example, consider a collection of images in which each image has a different width and height. It is unclear how to model such inputs with a weight matrix of fixed size. Convolution is straightforward to apply; the kernel is simply applied a different number of times depending on the size of the input, and the output of the convolution operation scales accordingly. Convolution may be viewed as matrix multiplication; the same convolution kernel induces a different size of doubly block circulant matrix for each size of input. Sometimes the output of the network as well as the input is allowed to have variable size, for example, if we want to assign a class label to each pixel of the input. In this case, no further design work is necessary. In other cases, the network must produce some fixed-size output, for example, if we want to assign a single class label to the entire image. In this case, we must make some additional design steps, like inserting a pooling layer whose pooling regions scale in size proportional to the size of the input, to maintain a fixed number of pooled outputs. Some examples of this kind of strategy are shown in figure 9.11.

Note that the use of convolution for processing variably sized inputs makes sense only for inputs that have variable size because they contain varying amounts of observation of the same kind of thing—different lengths of recordings over time, different widths of observations over space, and so forth. Convolution does not make sense if the input has variable size because it can optionally include different kinds of observations. For example, if we are processing college applications, and our features consist of both grades and standardized test scores, but not every applicant took the standardized test, then it does not make sense to convolve the same weights over features corresponding to the grades as well as the features

	Single channel	Multichannel
1-D	Audio waveform: The axis we	Skeleton animation data: Anima-
	convolve over corresponds to	tions of 3-D computer-rendered
	time. We discretize time and	characters are generated by alter-
	measure the amplitude of the	ing the pose of a "skeleton" over
	waveform once per time step.	time. At each point in time, the
		pose of the character is described
		by a specification of the angles of
		each of the joints in the charac-
		ter's skeleton. Each channel in
		the data we feed to the convolu-
		tional model represents the angle
		about one axis of one joint.
2-D	Audio data that has been prepro-	Color image data: One channel
	cessed with a Fourier transform:	contains the red pixels, one the
	We can transform the audio wave-	green pixels, and one the blue
	form into a 2-D tensor with dif-	pixels. The convolution kernel
	ferent rows corresponding to dif-	moves over both the horizontal
	ferent frequencies and different	and the vertical axes of the im-
	columns corresponding to differ-	age, conferring translation equiv-
	ent points in time. Using convolu-	ariance in both directions.
	tion in the time makes the model	
	equivariant to shifts in time. Using convolution across the fre-	
	quency axis makes the model	
	equivariant to frequency, so that	
	the same melody played in a dif-	
	ferent octave produces the same	
	representation but at a different	
	height in the network's output.	
3-D	Volumetric data: A common	Color video data: One axis corre-
Ü 2	source of this kind of data is med-	sponds to time, one to the height
	ical imaging technology, such as	of the video frame, and one to
	CT scans.	the width of the video frame.
	ı	

Table 9.1: Examples of different formats of data that can be used with convolutional networks.

corresponding to the test scores.

9.8 Efficient Convolution Algorithms

Modern convolutional network applications often involve networks containing more than one million units. Powerful implementations exploiting parallel computation resources, as discussed in section 12.1, are essential. In many cases, however, it is also possible to speed up convolution by selecting an appropriate convolution algorithm.

Convolution is equivalent to converting both the input and the kernel to the frequency domain using a Fourier transform, performing point-wise multiplication of the two signals, and converting back to the time domain using an inverse Fourier transform. For some problem sizes, this can be faster than the naive implementation of discrete convolution.

When a d-dimensional kernel can be expressed as the outer product of d vectors, one vector per dimension, the kernel is called **separable**. When the kernel is separable, naive convolution is inefficient. It is equivalent to compose d one-dimensional convolutions with each of these vectors. The composed approach is significantly faster than performing one d-dimensional convolution with their outer product. The kernel also takes fewer parameters to represent as vectors. If the kernel is w elements wide in each dimension, then naive multidimensional convolution requires $O(w^d)$ runtime and parameter storage space, while separable convolution requires $O(w \times d)$ runtime and parameter storage space. Of course, not every convolution can be represented in this way.

Devising faster ways of performing convolution or approximate convolution without harming the accuracy of the model is an active area of research. Even techniques that improve the efficiency of only forward propagation are useful because in the commercial setting, it is typical to devote more resources to deployment of a network than to its training.

9.11 Convolutional Networks and the History of Deep Learning

Convolutional networks have played an important role in the history of deep learning. They are a key example of a successful application of insights obtained by studying the brain to machine learning applications. They were also some of the first deep models to perform well, long before arbitrary deep models were considered viable. Convolutional networks were also some of the first neural networks to solve important commercial applications and remain at the forefront of commercial applications of deep learning today. For example, in the 1990s, the neural network research group at AT&T developed a convolutional network for reading checks (LeCun et al., 1998b). By the end of the 1990s, this system deployed by NCR was reading over 10 percent of all the checks in the United States. Later, several OCR and handwriting recognition systems based on convolutional nets were deployed by Microsoft (Simard et al., 2003). See chapter 12 for more details on such applications and more modern applications of convolutional networks. See LeCun et al. (2010) for a more in-depth history of convolutional networks up to 2010.

Convolutional networks were also used to win many contests. The current intensity of commercial interest in deep learning began when Krizhevsky et al.

(2012) won the ImageNet object recognition challenge, but convolutional networks had been used to win other machine learning and computer vision contests with less impact for years earlier.

Convolutional nets were some of the first working deep networks trained with back-propagation. It is not entirely clear why convolutional networks succeeded when general back-propagation networks were considered to have failed. It may simply be that convolutional networks were more computationally efficient than fully connected networks, so it was easier to run multiple experiments with them and tune their implementation and hyperparameters. Larger networks also seem to be easier to train. With modern hardware, large fully connected networks appear to perform reasonably on many tasks, even when using datasets that were available and activation functions that were popular during the times when fully connected networks were believed not to work well. It may be that the primary barriers to the success of neural networks were psychological (practitioners did not expect neural networks to work, so they did not make a serious effort to use neural networks). Whatever the case, it is fortunate that convolutional networks performed well decades ago. In many ways, they carried the torch for the rest of deep learning and paved the way to the acceptance of neural networks in general.

Convolutional networks provide a way to specialize neural networks to work with data that has a clear grid-structured topology and to scale such models to very large size. This approach has been the most successful on a two-dimensional image topology. To process one-dimensional sequential data, we turn next to another powerful specialization of the neural networks framework: recurrent neural networks.