Chapter 2

Neural Networks as Graphs

There is no rigorous definition of what deep learning is and what it is not. In fact, at the time of writing this, there is a raging debate in the artificial intelligence community about a clear definition. In this chapter, we will define neural networks generically as graphs of operations over real numbers. In practice, the shape of those graphs, called the *architecture*, is not arbitrary: Researchers and practitioners carefully construct new architectures to suit various tasks. For example, neural networks for image recognition typically look different from those for natural language tasks.

First, we will informally introduce graphs and look at some popular architectures. Then, we will formally define graphs and their semantics.

2.1 The Neural Building Blocks

A neural network is a graph where each node performs an operation. Overall, the graph represents a function from real numbers to real numbers, that is, $\mathbb{R}^n \to \mathbb{R}^m$. Consider the following very simple graph. The red node is an

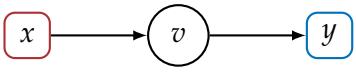


Figure 2.1 A very simple network

input node; it just passes input x, a real number, to node v. Node v performs some operation on x and spits out a value that goes to the *output* node y. For example, v might simply return $2x + 1$, which we will denote as the function

$f_v : \mathbb{R} \to \mathbb{R}$:

$$f_v(x) = 2x + 1$$

In our model, the output node may also perform some operation, for example,

$$f_y(x) = \max(0, x)$$

Taken together, this simple graph encodes the following function $f : \mathbb{R} \to \mathbb{R}$:

$$f(x) = f_y(f_v(x)) = \max(0, 2x + 1)$$

Transformations and Activations

The function f_v is an *affine transformation*. Simply, it multiplies inputs by constant values (in this case, $2x$) and adds constant values (1). The function f_y is an *activation* function, because it turns on or off. When its input is negative, f_y outputs 0, otherwise it outputs its input. Specifically, f_y is called a *rectified linear unit* (ReLU), and it is a very popular activation function in modern deep neural networks.

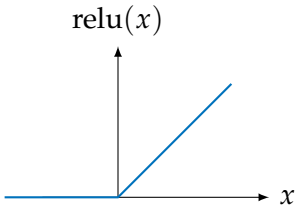


Figure 2.2 Rectified linear unit

There are other popular activation functions, for example, sigmoid,

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

whose output is bounded between 0 and 1, as shown in Figure 2.3.

Often, in the literature and practice, the affine transformation and the activation function are combined into a single operation. Our graph model of neural networks can capture that, but we usually prefer to distribute the two operations on two different nodes of the graph as it will simplify our life in later chapters when we start analyzing those graphs.

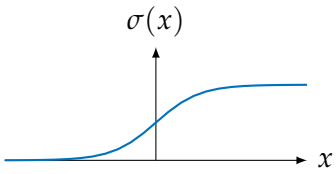


Figure 2.3 Sigmoid activation function

Universal approximation

What is so special about these activation functions? The short answer is they work in practice, in that they result in neural networks that are able to learn complex tasks. It is also very interesting to point out that you can construct a neural network comprised of ReLUs or sigmoids and affine transformations to approximate any function. This is known as the *universal approximation theorem*, and in fact the result is way more general than ReLUs and sigmoids—nearly any activation function you can think of works, as long as it is not polynomial!

2.2 Layers and Layers and Layers

In general, a neural network can be a crazy graph, with nodes and arrows pointing all over the place. In practice, networks are usually *layered*. Take the graph in Figure 2.4. Here we have 3 inputs and 3 outputs, $\mathbb{R}^3 \to \mathbb{R}^3$.

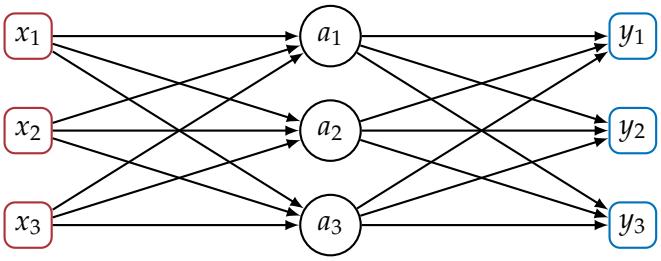


Figure 2.4 A multilayer perceptron

Notice that the nodes of the graph form layers, the input layer, the output

layer, and the layer in the middle which is called the *hidden* layer. This form of graph—or architecture—has the grandiose name of *multilayer perceptron* (MLP). Usually, we have a bunch of hidden layers in an MLP, like in Figure 2.5. Layers in an MLP are called *fully connected* layers, since each node

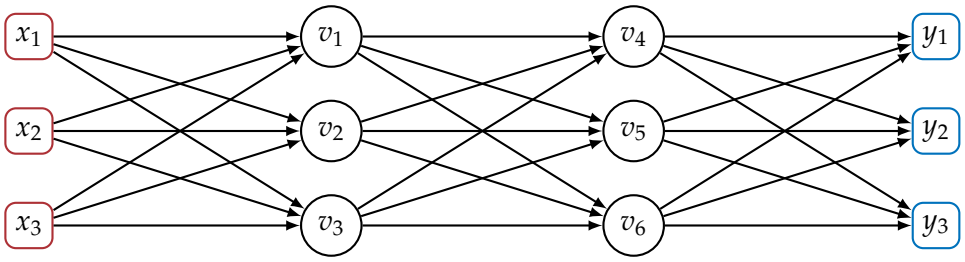


Figure 2.5 A multilayer perceptron with two hidden layers

receives all outputs from the preceding layer.

When we are doing classification, the output layer of the MLP represents the probability of each class, for example, y_1 is the probability of the input being a chair, y_2 is the probability of a TV, and y_3 of a couch. To ensure that the probabilities are normalized, that is, between 0 and 1 and sum up to 1, the final layer employs a *softmax* function. Softmax, generically, looks like this for an output node y_i, where n is the number of classes:

$$f_{y_i}(x_1, \ldots, x_n) = \frac{\exp(x_i)}{\sum_{k=1}^{n} \exp(x_k)}$$

To visualize why this actually works, please see Nielsen (2018, Chapter 3).

2.3 Convolutional Layers

Another kind of layer that you will find in a neural network is a *convolutional* layer. This kind of layer is widely used in computer vision tasks, but also has uses in natural language processing. The rough intuition is that if you are looking at an image, you want to scan it looking for patterns—the same thing is true of sentences in natural language. The convolutional layer gives you that: it defines an operation, a *kernel*, that is applied to every region of pixels in an image or every sequence of words in a sentence. For illustration,

let us consider an input layer of size 4, perhaps each input defines a word in a 4-word sentence, as shown in Figure 2.6. Here we have a kernel, nodes v_i, that is applied to every pair of consecutive words, $(x_1, x_2), (x_2, x_3)$, and (x_3, x_4). We say that this kernel has size 2, since it takes an input in $\mathbb{R}^2$. This kernel is 1-dimensional, since its input is a vector of real numbers. In practice, we work with 2-dimensional kernels or more; for instance, to scan blocks of pixels of a gray scale image where every pixel is a real number, we can use kernels that are functions in $\mathbb{R}^{10\times 10} \to \mathbb{R}$, meaning that the kernel is applied to every 10×10 sub-image in the input.

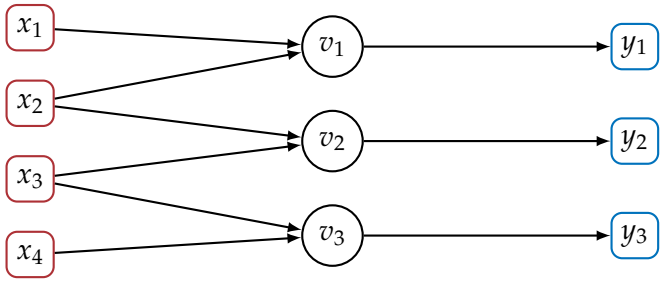


Figure 2.6 1-dimensional convolution

Typically, a *convolutional neural network* will apply a bunch of kernels to an input—and many layers of them—and aggregate (*pool*) the information from each kernel. We will formally define these operations in later chapters when we verify properties of such networks.

2.4 Where are the Loops?

All the neural networks we have seen so far seem to be a composition of a number mathematical functions, one after the other. So what about loops? Can we have loops in neural networks? In practice, neural network graphs are really just directed acyclic graphs (DAGs). This makes training the neural network possible using the *backpropagation* algorithm.

That said, there are popular classes of neural networks that appear to have loops, but they are very simple, in the sense that the number of iterations of the loop is just the size of the input. *Recurrent neural networks* (RNNs)

is the canonical class of such networks, which are usually used for sequence data, like text. You will often see the graph of an RNN rendered as follows, with the self loop on node v.

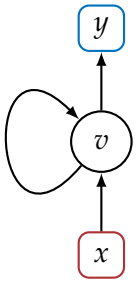


Figure 2.7 Recurrent neural network

Effectively, this graph represents an infinite family of acyclic graphs that unroll this loop a finite number of times. For example, the following is an unrolling of length 3. Notice that this is an acyclic graph that takes 3 inputs. The idea is that if you receive a sentence, say, with n words, you unroll the RNN to length n and apply it to the sentence.

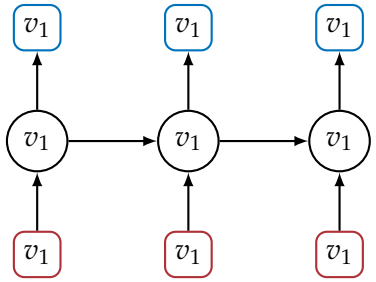


Figure 2.8 Unrolled recurrent neural network

Thinking of it through a programming lens, given an input, we can easily statically determine—i.e., without executing the network—how many loop iterations it will require. This is in contrast to, say, a program where the number of loop iterations is a complex function of its input, and therefore we do not know how many loop iterations it will take until we actually run

it. With this in mind, in what follows, we will formalize neural networks as acyclic graphs.

2.5 Structure and Semantics of Networks

We are done with looking at pretty graphs. Let us now look at pretty symbols. We will now formally define graphs and discuss some of their properties.

Networks as DAGs

A neural network is a directed acyclic graph $G = (V, E)$, where

- V is a finite set of nodes.
- $E \subseteq V \times V$ is a set of edges.
- $V^{\text{in}} \subseteq V$ is a non-empty set of input nodes.
- $V^{\circ} \subset V$ is a non-empty set of output nodes.
- Each non-input node v is associated with a function $f_v : \mathbb{R}^n \to \mathbb{R}$, where n is the number of edges whose target is v. Notice that we assume, for simplicity but without loss of generality, that a node v only outputs a single real value. The vector of real values $\mathbb{R}^n$ that v takes as input is all the outputs of nodes v' such that $(v', v) \in E$.

To make sure that a graph G does not have any dangling nodes and that semantics are clearly defined, we will assume the following structural properties:

- All nodes are reachable, via directed edges, from some input node.
- Every node can reach an output node.
- There is fixed total ordering on edges E and another one on nodes V.

Semantics of DAGs

A network $G = (V, E)$ defines a function in $\mathbb{R}^n \to \mathbb{R}^m$ where

$$n = |V^{\mathsf{in}}| \qquad m = |V^{\mathsf{o}}|$$

That is, G maps the values of the input nodes to those of the output nodes.

Specifically, for every non-input node $v \in V$, we recursively define the value in $\mathbb{R}$ that it produces as follows. Let $(v_1, v), \ldots, (v_n, v)$ be an ordered sequence of all edges whose target is v. Then,

$$\mathsf{out}(v) = f_v(x_1, \ldots, x_n)$$

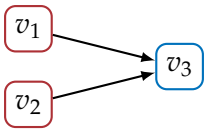
where $x_i = \mathsf{out}(v_i)$, for $i \in [1, n]$.

The base case of this definition is input nodes, since they have no edges incident on them. Suppose we are given an input $\boldsymbol{x} \in \mathbb{R}^n$, where we will use $\boldsymbol{x}$ to denote a vector and x_i to denote its ith element. Let $v_1, \ldots, v_n$ be an ordered sequence of all input nodes. Then,

$$\mathsf{out}(v_i) = x_i$$

A simple example

Let us look at an example graph G



We have $V^{\mathsf{in}} = \{v_1, v_2\}$ and $V^{\mathsf{o}} = \{v_3\}$. Now assume that

$$f_{v_3}(x_1, x_2) = x_1 + x_2$$

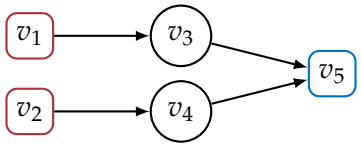
and that we are given the input vector $(11, 79)$ to the network, where node v_1 gets the value 11 and v_2 the value 79. Then, we have

$$\begin{aligned}
&\mathsf{out}(v_1) = 11 \\
&\mathsf{out}(v_2) = 79 \\
&\mathsf{out}(v_3) = \mathsf{out}(v_1) + \mathsf{out}(v_2) = 11 + 79 = 90
\end{aligned}$$

Data flow and control flow

The graphs we have defined are known in the field of program analysis as *data-flow* graphs; this is in contrast to *control-flow* graphs.[1] Control-flow graphs dictate the *order* in which operations need be performed—the flow of who has *control* of the CPU. Data-flow graphs, on the other hand, only tell us what node needs what data to perform its computation, but not how to order the computation. This is best seen through a small example.

Consider the following graph



Viewing this graph as an imperative program, one way to represent it is as follows, where $\leftarrow$ is the assignment symbol.

$$\begin{aligned}
\mathsf{out}(v_3) &\leftarrow f_{v_3}(\mathsf{out}(v_1)) \\
\mathsf{out}(v_4) &\leftarrow f_{v_4}(\mathsf{out}(v_2)) \\
\mathsf{out}(v_5) &\leftarrow f_{v_5}(\mathsf{out}(v_3), \mathsf{out}(v_4))
\end{aligned}$$

This program dictates that the value of v_3 is computed before v_4. But this need not be, as the output of one does not depend on the the other. Therefore, an equivalent implementation of the same graph can swap the first two operations:

$$\begin{aligned}
\mathsf{out}(v_4) &\leftarrow f_{v_4}(\mathsf{out}(v_2)) \\
\mathsf{out}(v_3) &\leftarrow f_{v_3}(\mathsf{out}(v_1)) \\
\mathsf{out}(v_5) &\leftarrow f_{v_5}(\mathsf{out}(v_3), \mathsf{out}(v_4))
\end{aligned}$$

Formally, we can compute the values $\mathsf{out}(\cdot)$ in any *topological* ordering of graph nodes. This ensures that all inputs of a node are computed before its own operation is performed.

[1] In deep learning frameworks like TensorFlow, they call graphs *computation graphs*.

Properties of operations

So far, we have assumed that a node v can implement any operation f_v it wants over real numbers. In practice, to enable efficient training of neural networks, these operations need be *differentiable* or differentiable *almost everywhere*. The ReLU activation function, Figure 2.2, that we have seen earlier is differentiable almost everywhere, since at $x = 0$, there is a sharp turn in the function and the gradient is undefined.

Many of the operations we will be concerned with are *linear* or *piecewise linear*. Formally, a function $f : \mathbb{R}^n \to \mathbb{R}$ is linear if it can be defined as follows:

$$f(\boldsymbol{x}) = \sum_i c_i x_i + b$$

where $c_i, b \in \mathbb{R}$. A function is piecewise linear if it can be written in the form

$$f(\boldsymbol{x}) = \begin{cases} \sum_i c_i^1 x_i + b^1, & \boldsymbol{x} \in S_1 \\ \vdots & \\ \sum_i c_i^m x_i + b^m, & \boldsymbol{x} \in S_m \end{cases}$$

where S_i are mutually disjoint subsets of $\mathbb{R}^n$ and $\cup_i S_i = \mathbb{R}^n$. ReLU, for instance, is a piecewise linear function, as it is of the form:

$$\text{relu}(x) = \begin{cases} 0, & x < 0 \\ x, & x \geqslant 0 \end{cases}$$

Another important property that we will later exploit is *monotonicity*. A function $f : \mathbb{R} \to \mathbb{R}$ is monotone if for any $x \geqslant y$, we have $f(x) \geqslant f(y)$. Both activation functions we saw earlier in the chapter, ReLUs and sigmoids, are monotone. You can verify this in Figures 2.2 and 2.3: the functions never decrease with increasing values of x.

Looking Ahead

Now that we have formally defined neural networks, we are ready to pose questions about their behavior. In the next chapter, we will formally define a language for posing those questions. Then, in the chapters that follow, we will look at algorithms for answering those questions.