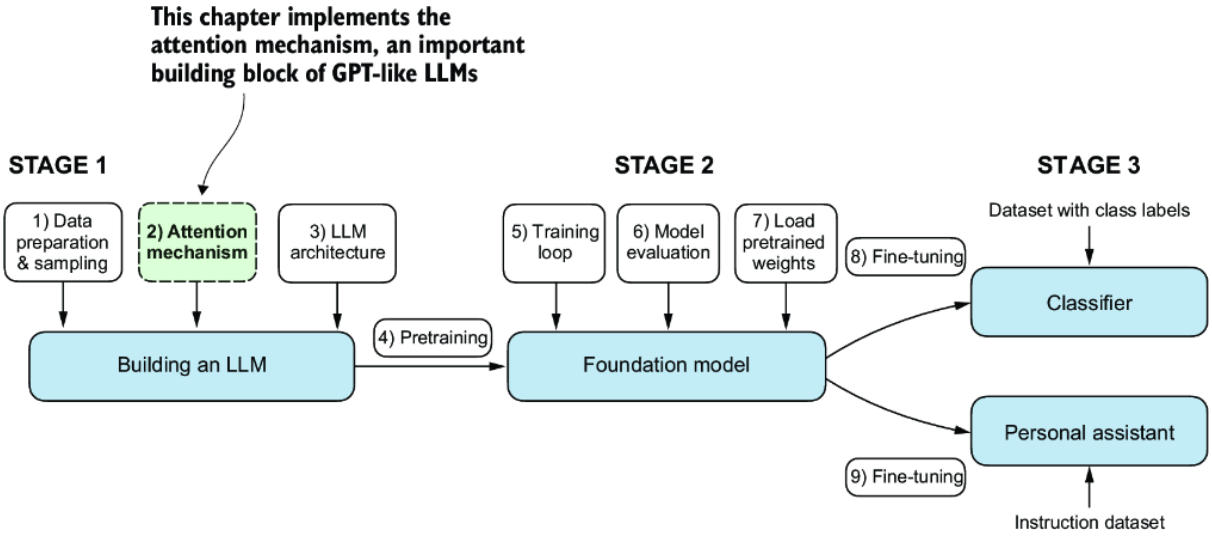
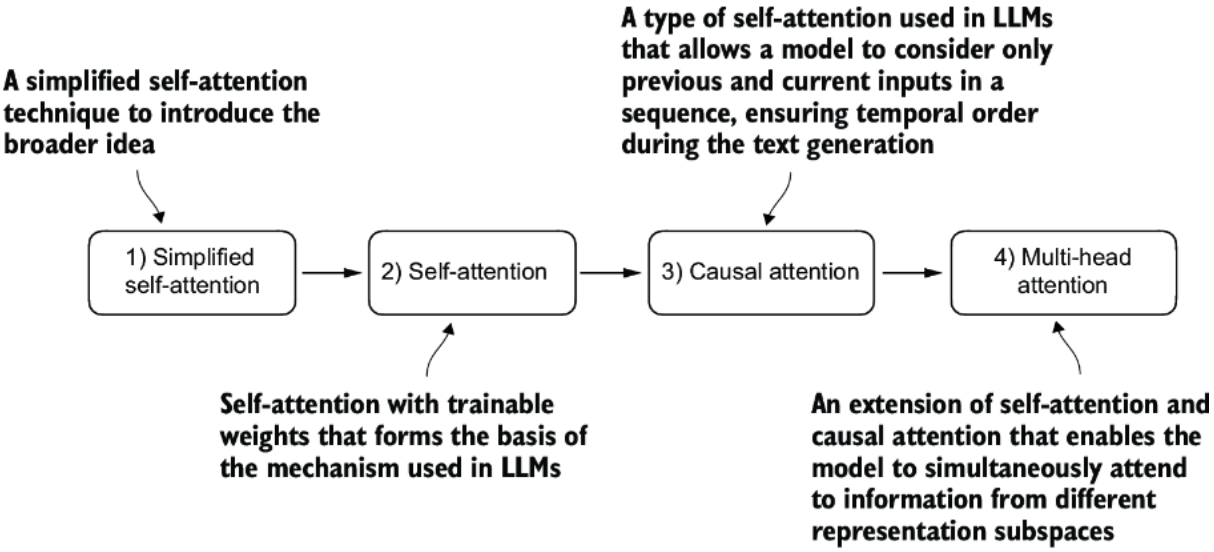
chapter 3

The three main stages of coding an LLM. This chapter focuses on step 2 of stage 1: implementing attention mechanisms, which are an integral part of the LLM architecture.

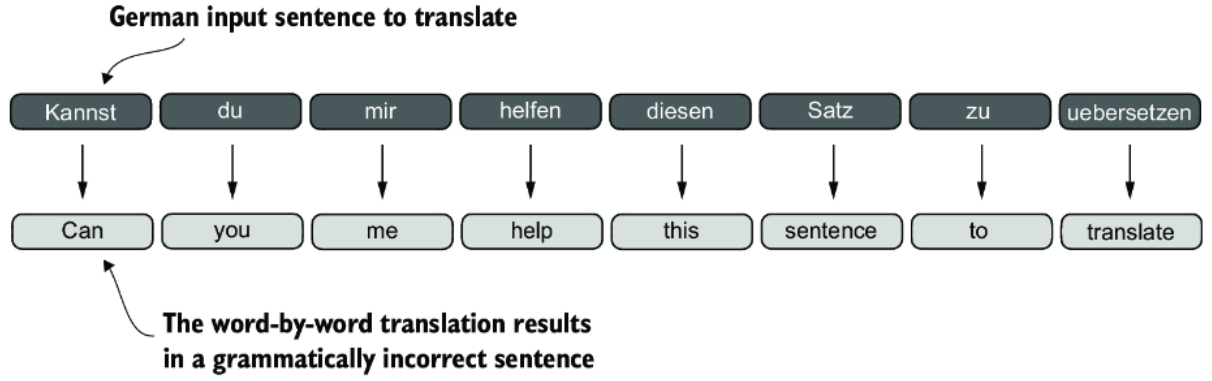


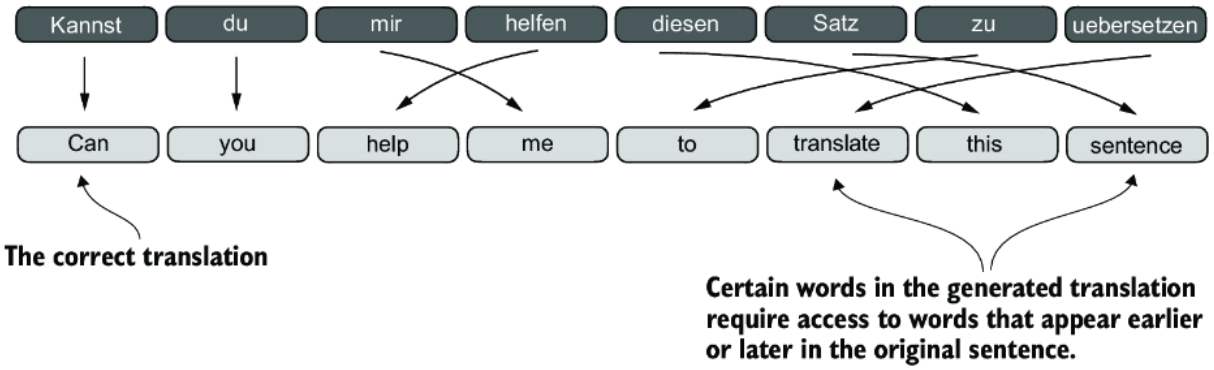
We will implement four different variants of attention mechanisms, as illustrated in the figure below. These different attention variants build on each other, and the goal is to arrive at a compact and efficient implementation of multi-head attention that we can then plug into the LLM architecture we will code in the next chapter.

The figure depicts different attention mechanisms we will code in this chapter, starting with a simplified version of self-attention before adding the trainable weights. The causal attention mechanism adds a mask to self-attention that allows the LLM to generate one word at a time. Finally, multi-head attention organizes the attention mechanism into multiple heads, allowing the model to capture various aspects of the input data in parallel.



When translating text from one language to another, such as German to English, it's not possible to merely translate word by word. Instead, the translation process requires contextual understanding and grammatical alignment.





Fortunately, it is not essential to understand RNNs to build an LLM. Just remember that encoder–decoder RNNs had a shortcoming that motivated the

design of attention mechanisms.

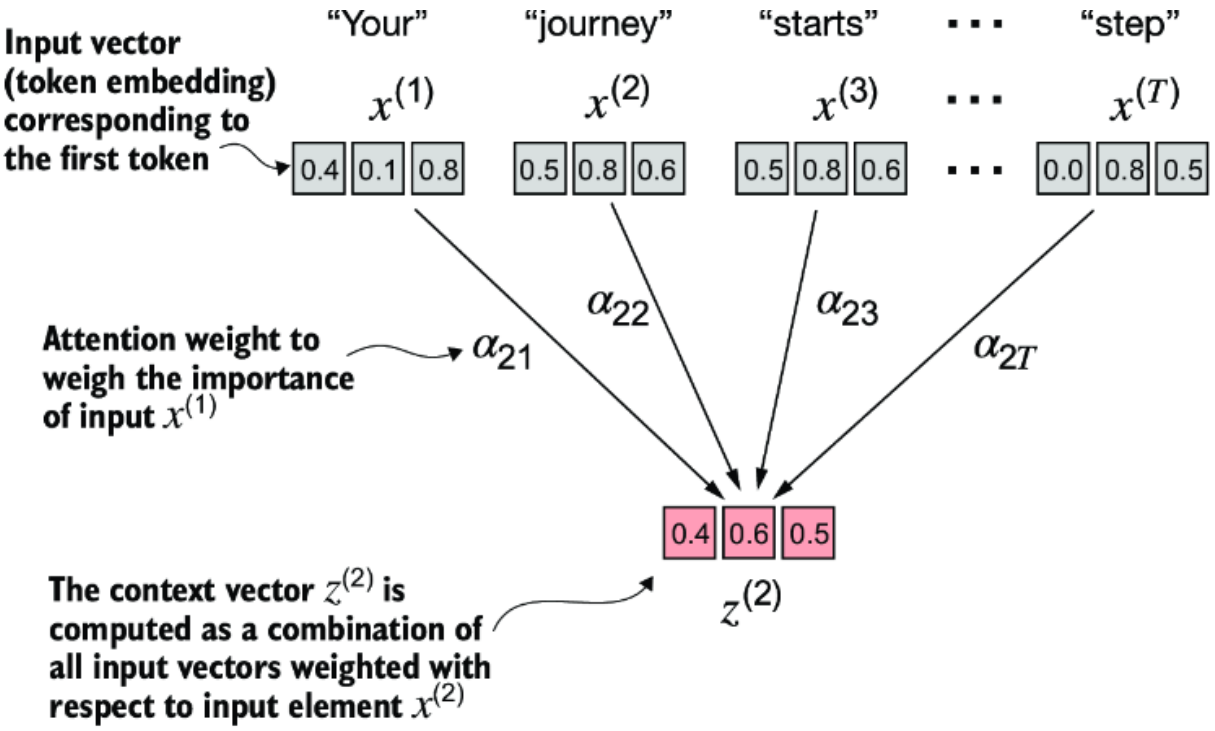
In self-attention, the “self” refers to the mechanism’s ability to compute attention weights by relating different positions within a single input sequence. It assesses and learns the relationships and dependencies between various parts of the input itself, such as words in a sentence or pixels in an image.

This is in contrast to traditional attention mechanisms, where the focus is on the relationships between elements of two different sequences, such as in sequence-to-sequence models where the attention might be between an input sequence and an output sequence.

A simple self-attention mechanism without trainable weights

Let’s begin by implementing a simplified variant of self-attention, free from any trainable weights, as summarized in figure 3.7. The goal is to illustrate a few key concepts in self-attention before adding trainable weights.

Figure 3.7 The goal of self-attention is to compute a context vector for each input element that combines information from all other input elements. In this example, we compute the context vector z(2). The importance or contribution of each input element for computing z(2) is determined by the attention weights a21 to a2T. When computing z(2), the attention weights are calculated with respect to input element x(2) and all other inputs.



For example, consider an input text like "Your journey starts with one step." In this case, each element of the sequence, such as *x*(1), corresponds to a *d*-dimensional embedding vector representing a specific token, like "Your." Figure 3.7 shows these input vectors as three-dimensional embeddings.

In self-attention, our goal is to calculate context vectors *z*(i) for each element *x*(i) in the input sequence. A *context vector* can be interpreted as an enriched embedding vector.

To illustrate this concept, let's focus on the embedding vector of the second input element, *x*(2) (which corresponds to the token "journey"), and the corresponding context vector, *z*(2), shown at the bottom of figure 3.7. This enhanced context vector, *z*(2), is an embedding that contains information about *x*(2) and all other input elements, *x*(1) to *x*(T).

Context vectors play a crucial role in self-attention. Their purpose is to create enriched representations of each element in an input sequence (like a sentence) by incorporating information from all other elements in the sequence (figure 3.7). This is essential in LLMs, which need to understand the relationship and relevance of words in a sentence to each other. Later, we will add trainable weights that help an LLM learn to construct these context vectors so that they are relevant for the LLM to generate the next token. But first, let's

implement a simplified self-attention mechanism to compute these weights and the resulting context vector one step at a time.

Consider the following input sentence, which has already been embedded into three-dimensional vectors (see chapter 2). I've chosen a small embedding dimension to ensure it fits on the page without line breaks:

```
import torch
inputs = torch.tensor(
  [[0.43, 0.15, 0.89], # Your     (x^1)
   [0.55, 0.87, 0.66], # journey  (x^2)
   [0.57, 0.85, 0.64], # starts   (x^3)
   [0.22, 0.58, 0.33], # with     (x^4)
   [0.77, 0.25, 0.10], # one      (x^5)
   [0.05, 0.80, 0.55]] # step     (x^6)
)
```

Figure 3.8 The overall goal is to illustrate the computation of the context vector z(2) using the second input element, x(2) as a query. This figure shows the first intermediate step, computing the attention scores w between the query x(2) and all other input elements as a dot product. (Note that the numbers are truncated to one digit after the decimal point to reduce visual clutter.)

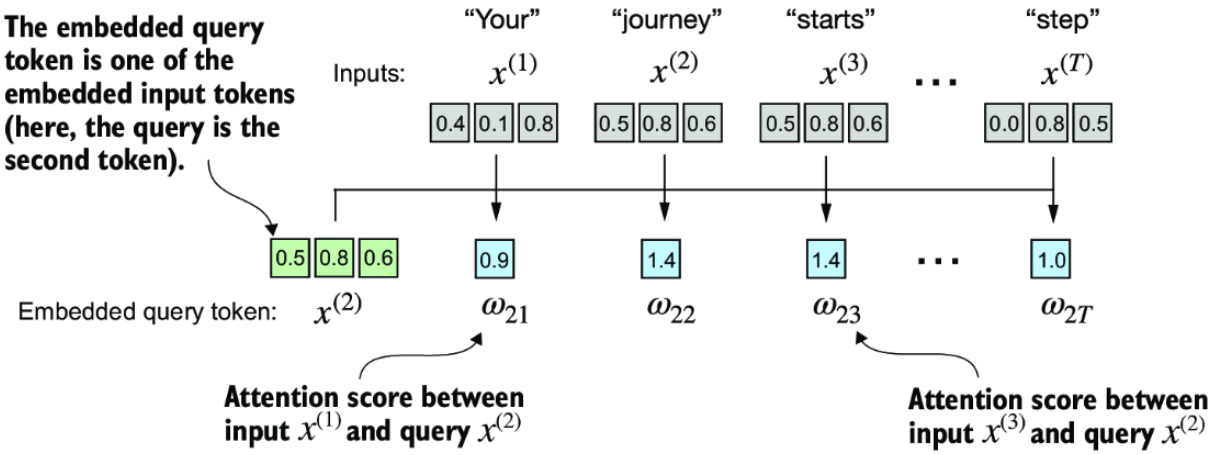


Figure 3.8 illustrates how we calculate the intermediate attention scores between the query token and each input token. We determine these scores by computing the dot product of the query, $x(2)$, with every other input token:

Understanding dot products

A dot product is essentially a concise way of multiplying two vectors element-wise and then summing the products

Beyond viewing the dot product operation as a mathematical tool that combines two vectors to yield a scalar value, the dot product is a measure of similarity because it quantifies how closely two vectors are aligned: a higher dot product indicates a greater degree of alignment or similarity between the vectors. In the context of self-attention mechanisms, the dot product determines the extent to which each element in a sequence focuses on, or “attends to,” any other element: the higher the dot product, the higher the similarity and attention score between two elements.

In the next step, as shown in figure 3.9, we normalize each of the attention scores we computed previously. The main goal behind the normalization is to obtain attention weights that sum up to 1. This normalization is a convention that is useful for interpretation and maintaining training stability in an LLM. Here’s a straightforward method for achieving this normalization step:

code...

In practice, it’s more common and advisable to use the softmax function for normalization. This approach is better at managing extreme values and offers more favorable gradient properties during training. The following is a basic implementation of the softmax function for normalizing the attention scores:

code...

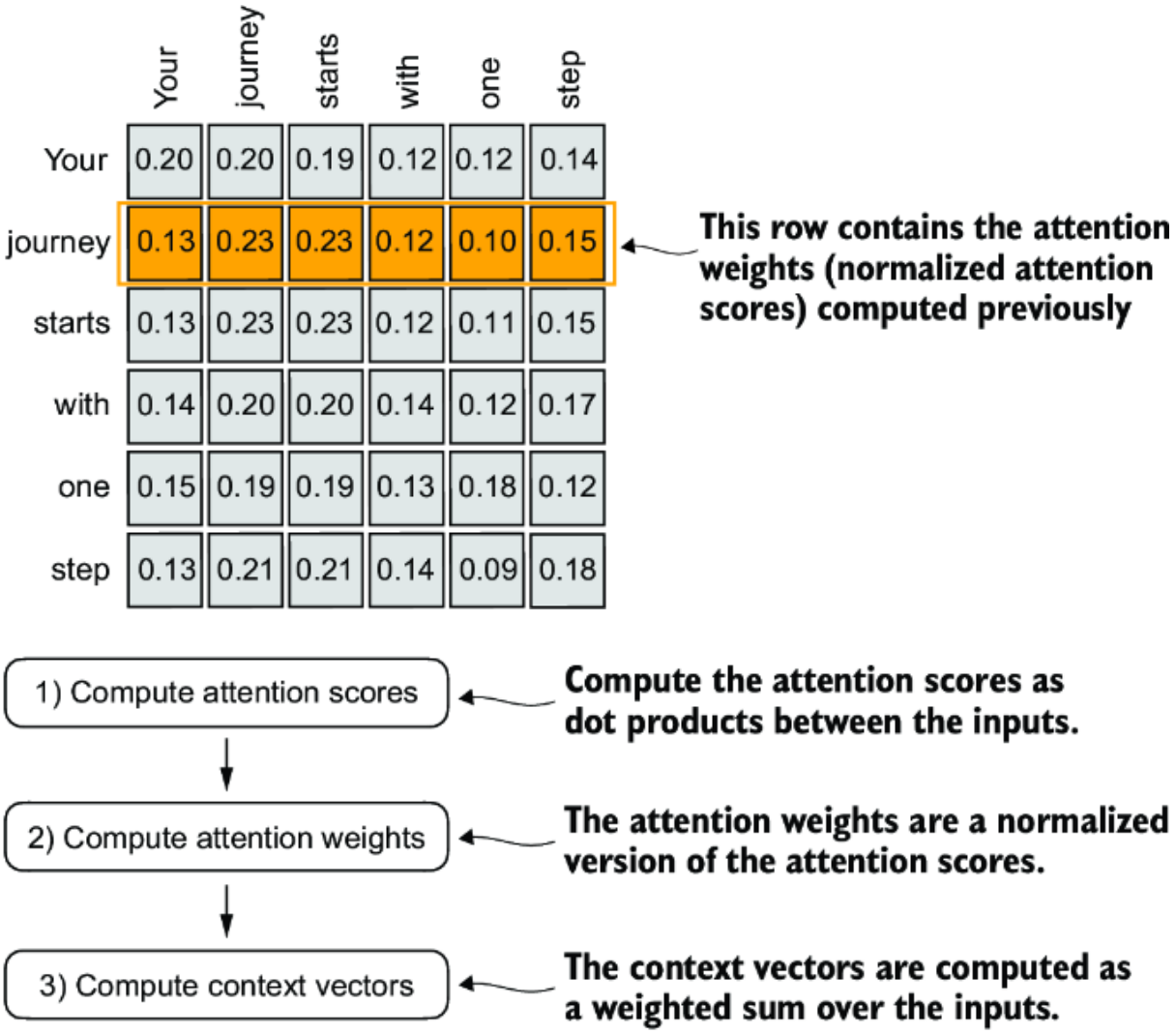
In addition, the softmax function ensures that the attention weights are always positive. This makes the output interpretable as probabilities or relative importance, where higher weights indicate greater importance.

Note that this naive softmax implementation (`softmax_naive`) may encounter numerical instability problems, such as overflow and underflow, when dealing with large or small input values. Therefore, in practice, it’s advisable to use the PyTorch implementation of softmax, which has been extensively optimized for performance:

Computing attention weights for all input tokens

So far, we have computed attention weights and the context vector for input 2, as shown in the highlighted row in figure 3.11. Now let’s extend this computation to calculate attention weights and context vectors for all inputs.

Figure 3.11 The highlighted row shows the attention weights for the second input element as a query. Now we will generalize the computation to obtain all other attention weights. (Please note that the numbers in this figure are truncated to two digits after the decimal point to reduce visual clutter. The values in each row should add up to 1.0 or 100%.)



When computing the preceding attention score tensor, we used `for` loops in Python. However, `for` loops are generally slow, and we can achieve the same results using matrix multiplication