EE 628
Deep Learning
Fall 2019

Lecture 11

11/07/2019

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STEVENS INSTITUTE of TECHNOLOGY

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Overview

- Last lecture we covered
  - Data Preparation for RNNs
  - Implementing RNNs from scratch

- Today, we will cover
  - Finish implementing RNN
  - GRUs and LSTMs
  - Attention Mechanism

Open notebook IN_CLASS_implementation_of_RNNs_from_scratch

Backpropagation Through Time

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- Forward propagation in a recurrent neural network is relatively straightforward.
- Back-propagation through time is actually a specific application of back propagation in recurrent neural networks.

The computation graph

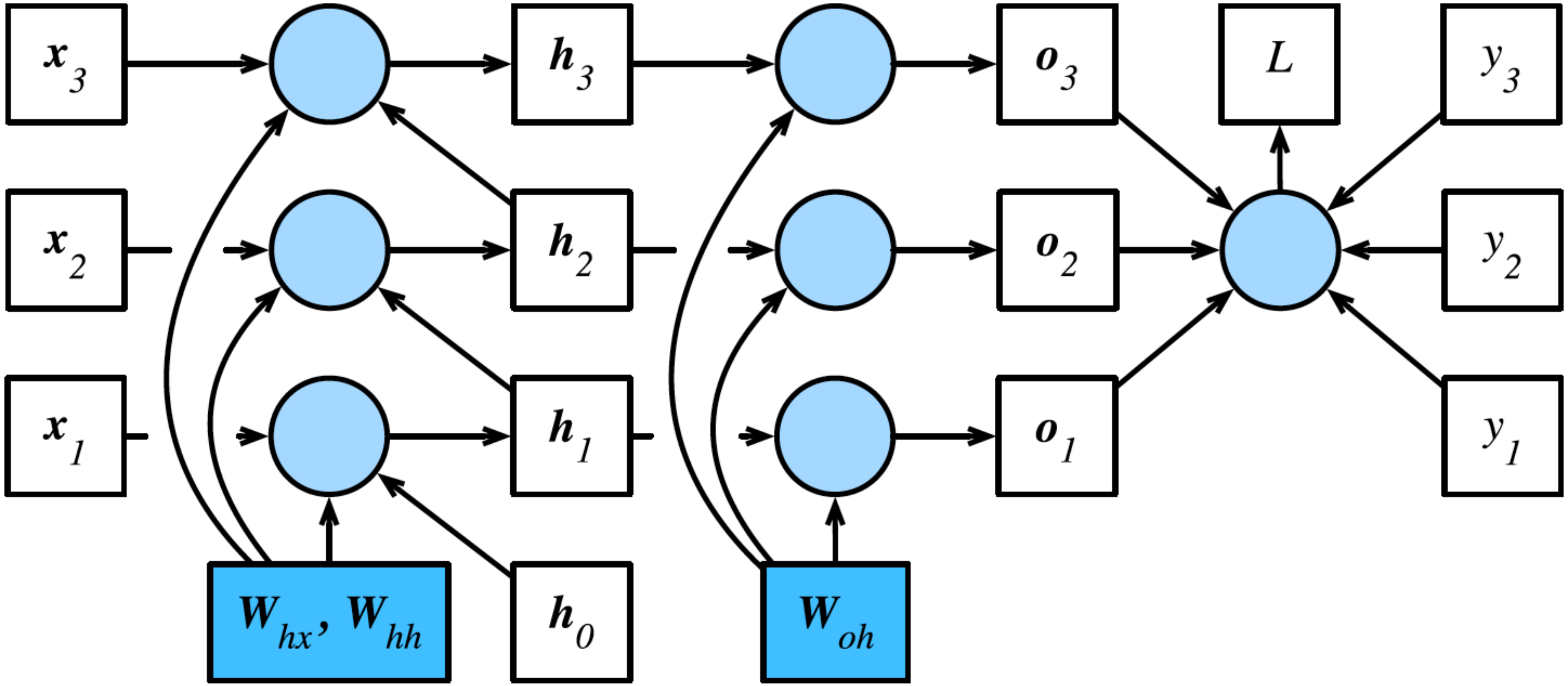

Fig. 10.7.2: Computational dependencies for a recurrent neural network model with three time steps. Boxes represent variables (not shaded) or parameters (shaded) and circles represent operators.

BPTT in detail

- In a simple linear latent variable model, we have:

$$\mathbf{h}_t = \mathbf{W}_{hx}\mathbf{x}_t + \mathbf{W}_{hh}\mathbf{h}_{t-1} \text{ and } \mathbf{o}_t = \mathbf{W}_{oh}\mathbf{h}_t$$

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  - This is numerically unstable and gives undue importance to potentially irrelevant past detail.
- One way to address this is to truncate the sum at a computationally convenient size.
  - That is why we detached the gradients in the code

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- The Gated Recurrent Unit (GRU) is a slightly more streamlined variant that often offers comparable performance and is significantly faster to compute.

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  - Lastly, we will learn to reset the latent state whenever needed.

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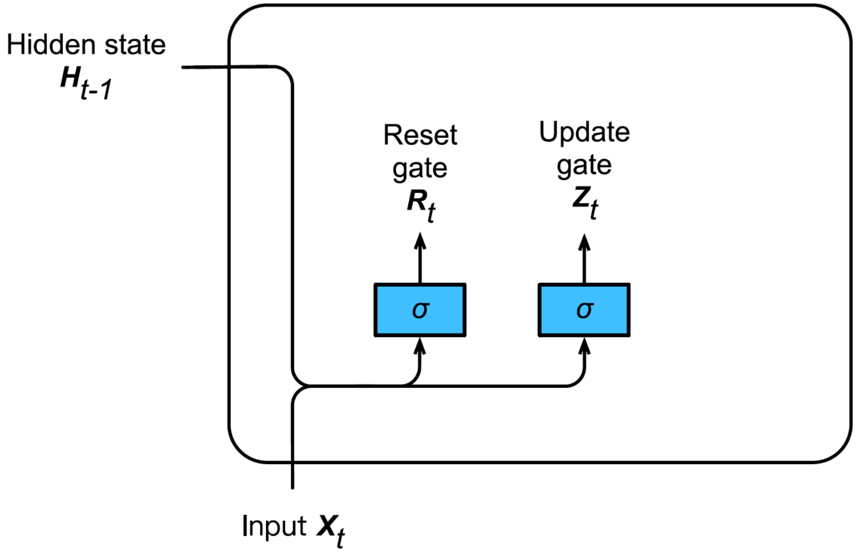

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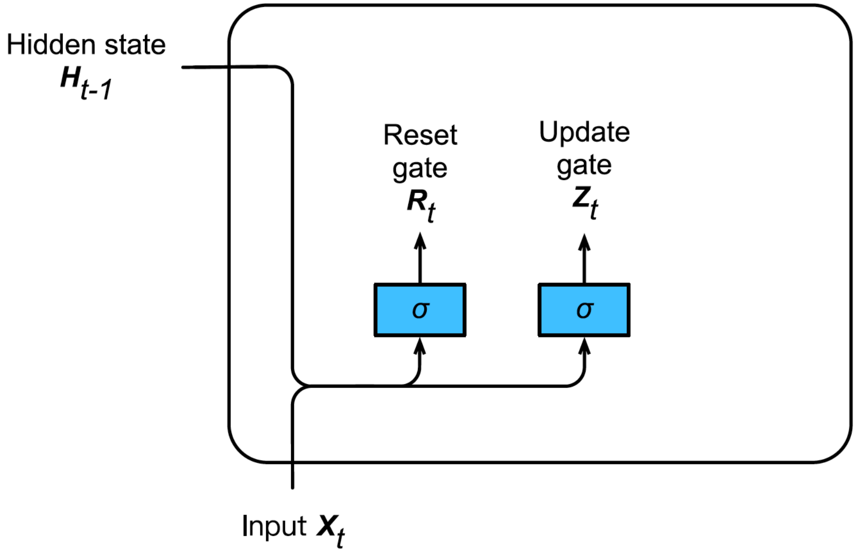

$$\mathbf{R}_t = \sigma(\mathbf{X}_t \mathbf{W}_{xr} + \mathbf{H}_{t-1} \mathbf{W}_{hr} + \mathbf{b}_r)$$
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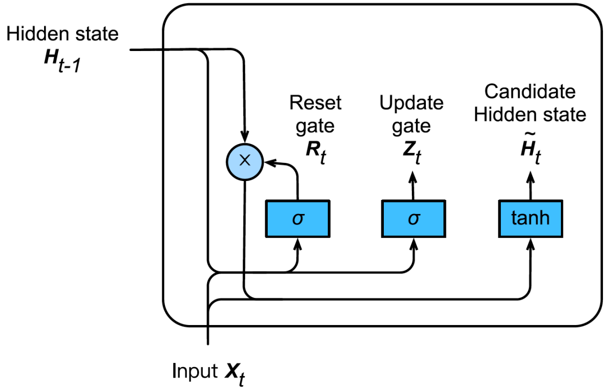

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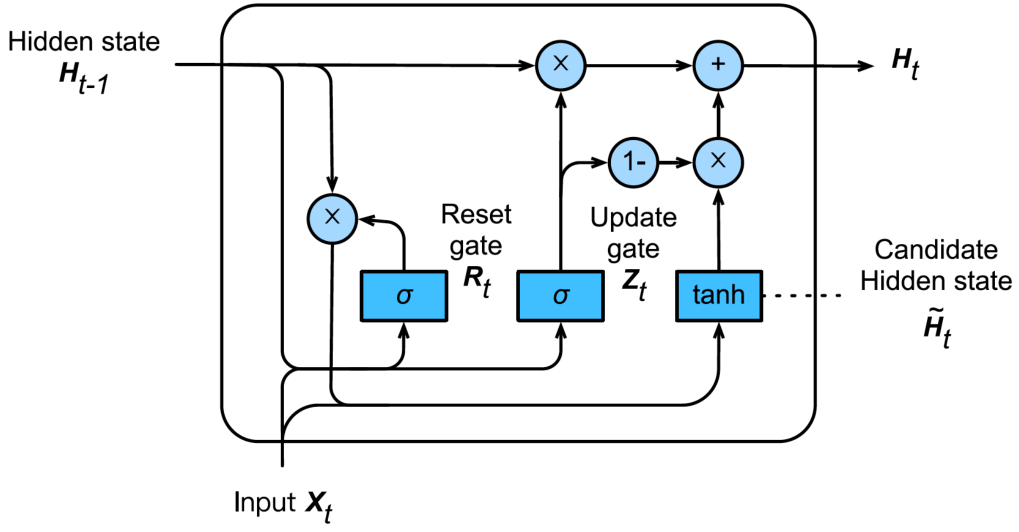

In summary

- GRUs have the following two distinguishing features:
  - Reset gates help capture short-term dependencies in time series.
  - Update gates help capture long-term dependencies in time series

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  - Lastly, we need a mechanism to reset the contents of the cell -> forget gate

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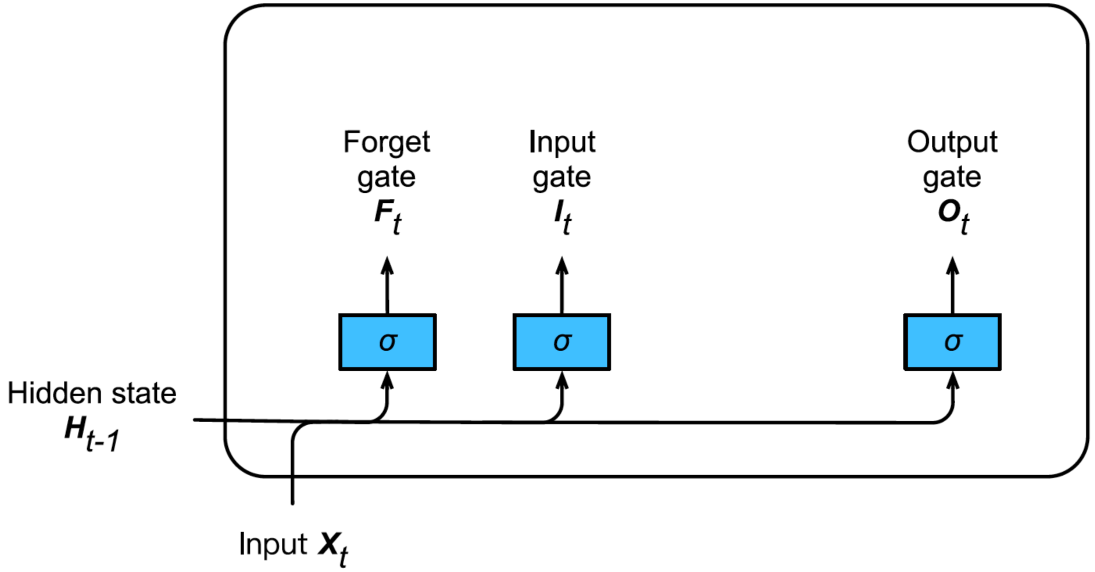

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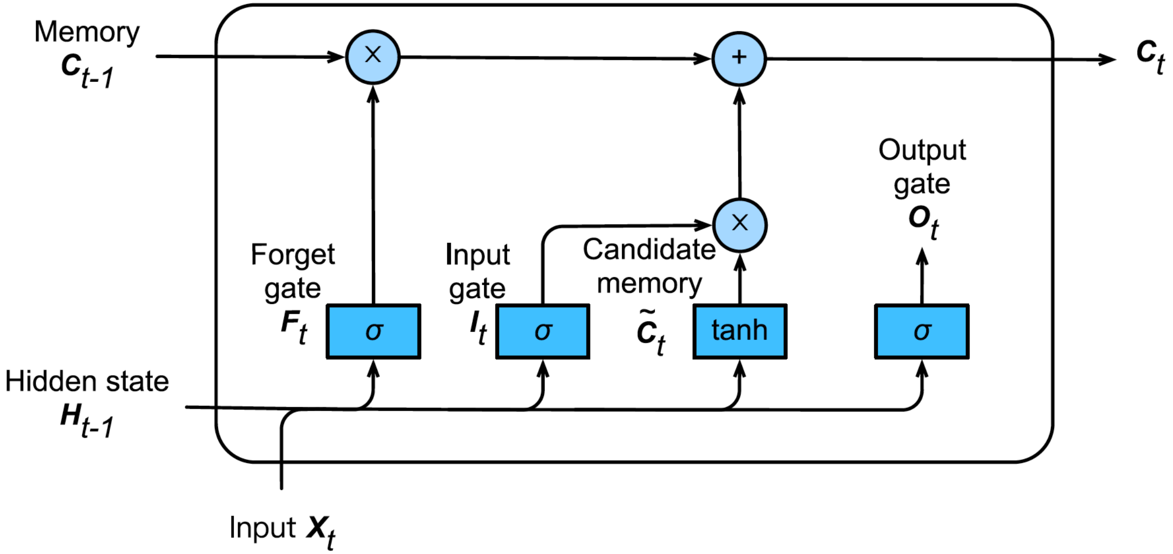

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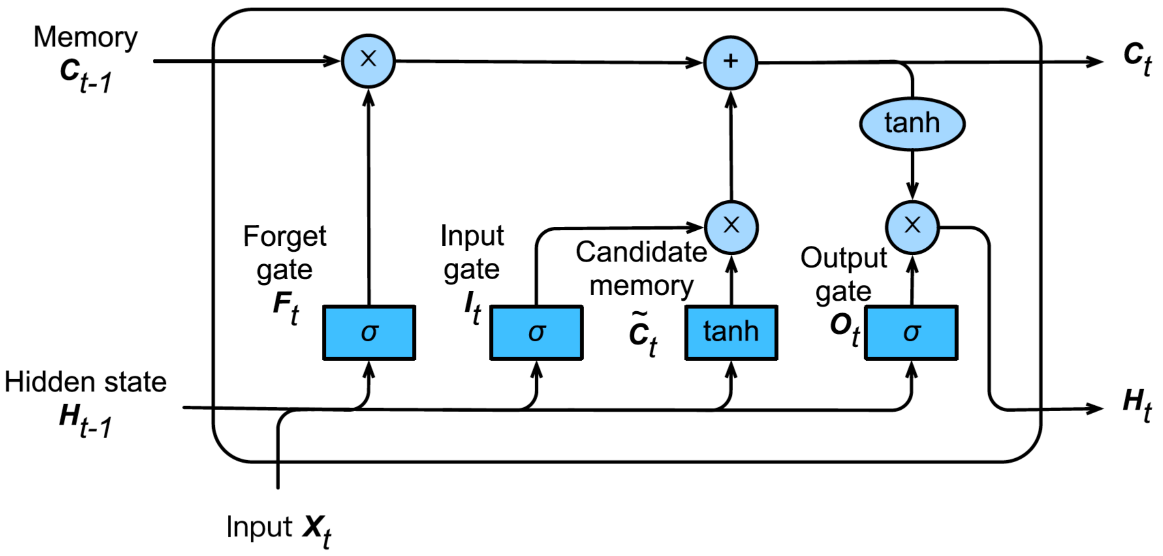

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$$\mathbf{H}_t^{(1)} = f_1\left(\mathbf{X}_t, \mathbf{H}_{t-1}^{(1)}\right)$$

$$\mathbf{H}_t^{(l)} = f_l\left(\mathbf{H}_t^{(l-1)}, \mathbf{H}_{t-1}^{(l)}\right)$$

$$\mathbf{O}_t = g\left(\mathbf{H}_t^{(L)}\right)$$

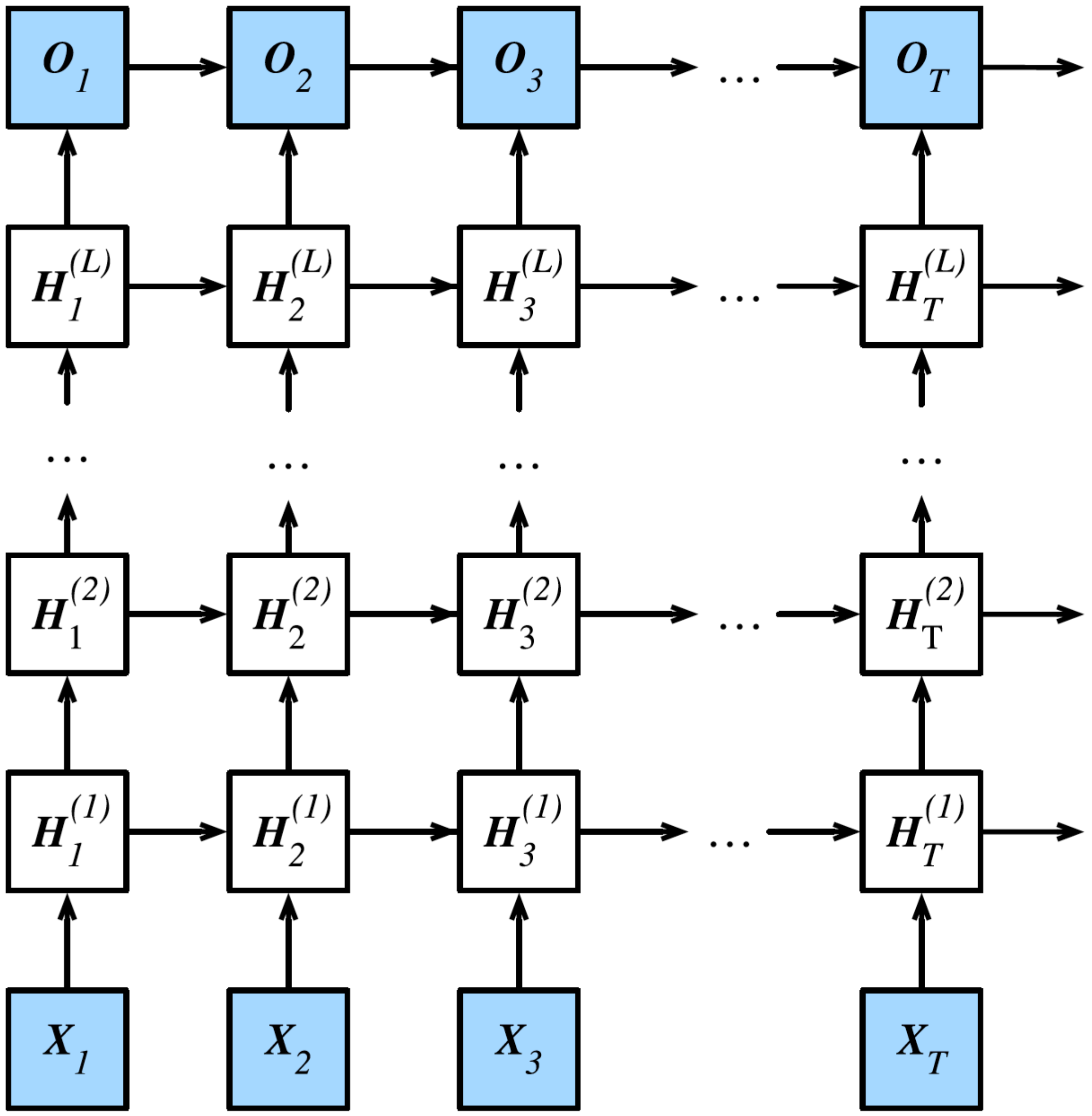
Deep Recurrent Neural Networks

- Consider a deep recurrent neural network with L hidden layers.
- Each hidden state is continuously passed to the next time step of the current layer and the next layer of the current time step.

$$\mathbf{H}_t^{(1)} = f_1\left(\mathbf{X}_t, \mathbf{H}_{t-1}^{(1)}\right)$$

$$\mathbf{H}_t^{(l)} = f_l\left(\mathbf{H}_t^{(l-1)}, \mathbf{H}_{t-1}^{(l)}\right)$$

$$\mathbf{O}_t = g\left(\mathbf{H}_t^{(L)}\right)$$



Bidirectional Recurrent Neural Networks

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- Clearly the end of the phrase (if available) conveys significant information about which word to pick.

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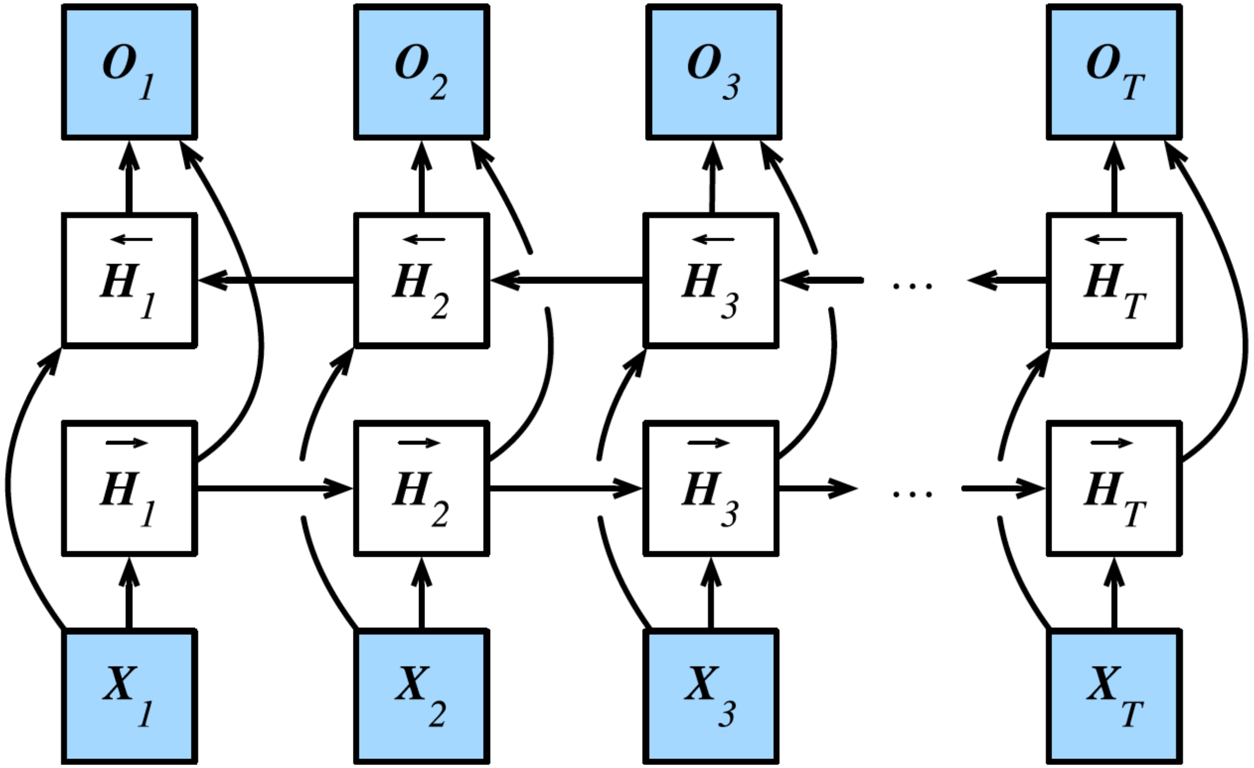

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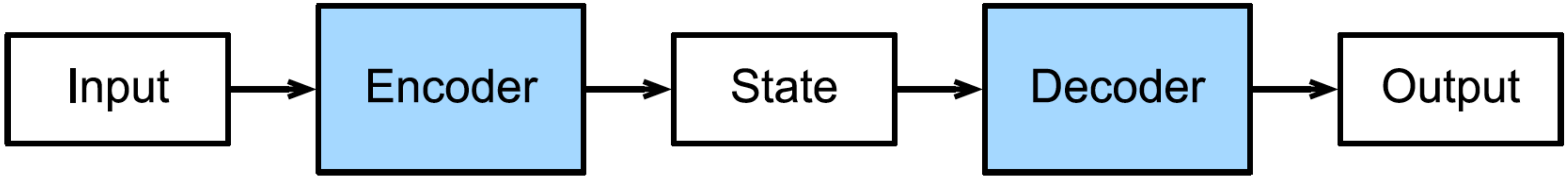

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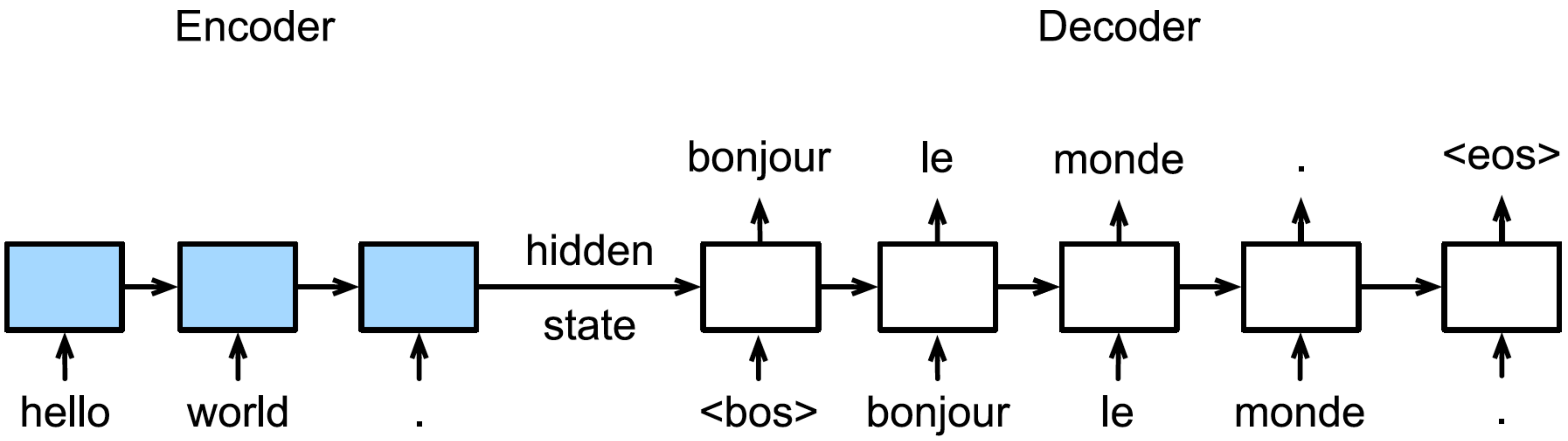

Fig. 10.14.1: The sequence to sequence model architecture.

Seq2SeqEncoder

```
# Saved in the d2l package for later use
class Seq2SeqEncoder(d2l.Encoder):
    def __init__(self, vocab_size, embed_size, num_hiddens, num_layers,
                 dropout=0, **kwargs):
        super(Seq2SeqEncoder, self).__init__(**kwargs)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        self.rnn = rnn.LSTM(num_hiddens, num_layers, dropout=dropout)

    def forward(self, X, *args):
        X = self.embedding(X) # X shape: (batch_size, seq_len, embed_size)
        X = X.swapaxes(0, 1)  # RNN needs first axes to be time
        state = self.rnn.begin_state(batch_size=X.shape[1], ctx=X.context)
        out, state = self.rnn(X, state)
        # The shape of out is (seq_len, batch_size, num_hiddens).
        # state contains the hidden state and the memory cell
        # of the last time step, the shape is (num_layers, batch_size, num_hiddens)
        return out, state
```

Seq2SeqEncoder

```
encoder = Seq2SeqEncoder(vocab_size=10, embed_size=8,
                         num_hiddens=16, num_layers=2)
encoder.initialize()
X = np.zeros((4, 7))
output, state = encoder(X)
output.shape, len(state), state[0].shape, state[1].shape
```

```
((7, 4, 16), 2, (2, 4, 16), (2, 4, 16))
```

Seq2SeqDecoder

```
# Saved in the d2l package for later use
class Seq2SeqDecoder(d2l.Decoder):
    def __init__(self, vocab_size, embed_size, num_hiddens, num_layers,
                 dropout=0, **kwargs):
        super(Seq2SeqDecoder, self).__init__(**kwargs)
        self.embedding = nn.Embedding(vocab_size, embed_size)
        self.rnn = rnn.LSTM(num_hiddens, num_layers, dropout=dropout)
        self.dense = nn.Dense(vocab_size, flatten=False)

    def init_state(self, enc_outputs, *args):
        return enc_outputs[1]

    def forward(self, X, state):
        X = self.embedding(X).swapaxes(0, 1)
        out, state = self.rnn(X, state)
        # Make the batch to be the first dimension to simplify loss computation.
        out = self.dense(out).swapaxes(0, 1)
        return out, state
```

Add dense layer with the hidden size to be the vocabulary size

Seq2SeqDecoder

```
decoder = Seq2SeqDecoder(vocab_size=10, embed_size=8,
                         num_hiddens=16, num_layers=2)
decoder.initialize()
state = decoder.init_state(encoder(X))
out, state = decoder(X, state)
out.shape, len(state), state[0].shape, state[1].shape
```

```
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Attention Mechanism

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- The attention mechanism, however, makes this selection explicit.

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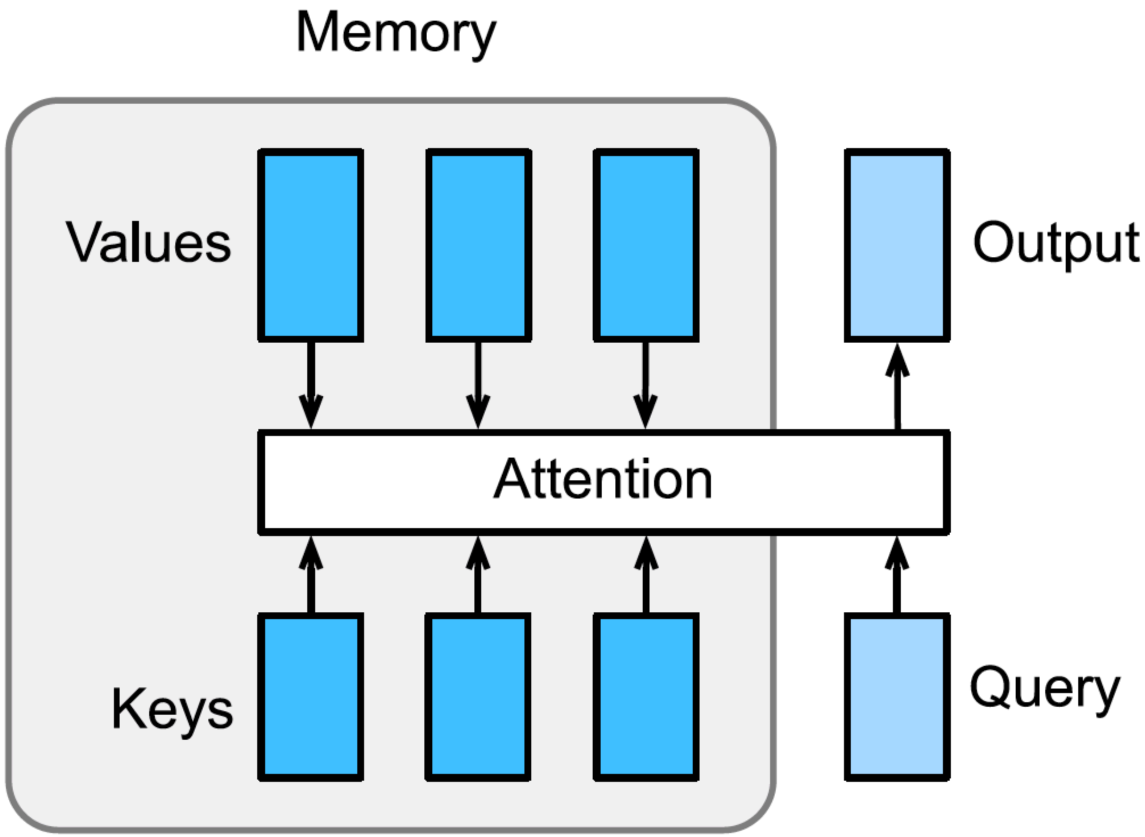

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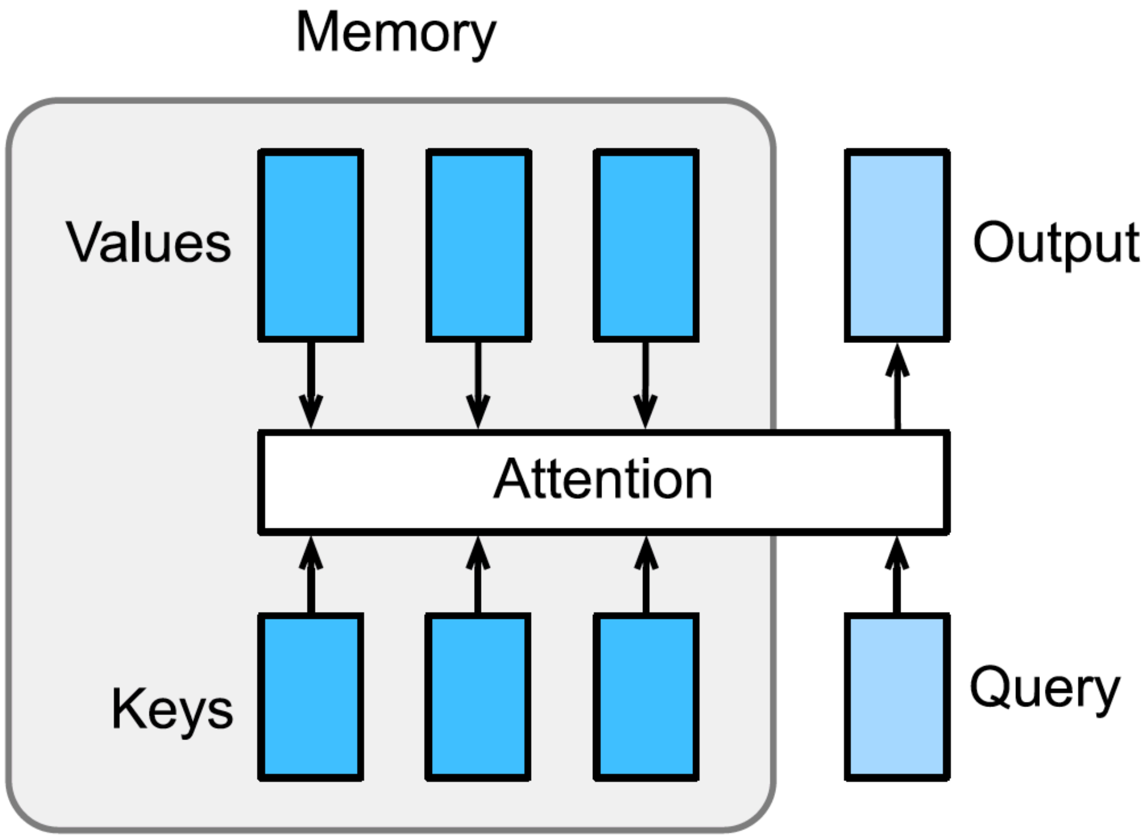

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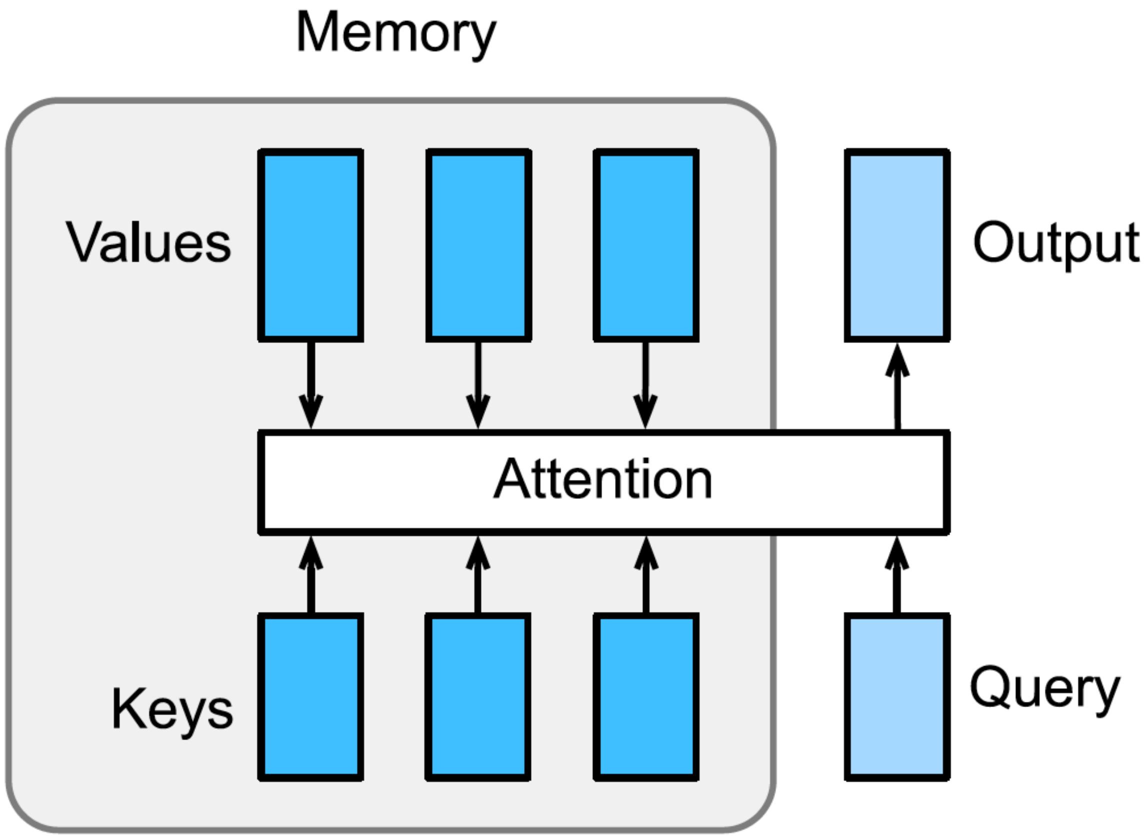
- For a query, the attention layer returns the output based on its memory, which is a set of key-value pairs.



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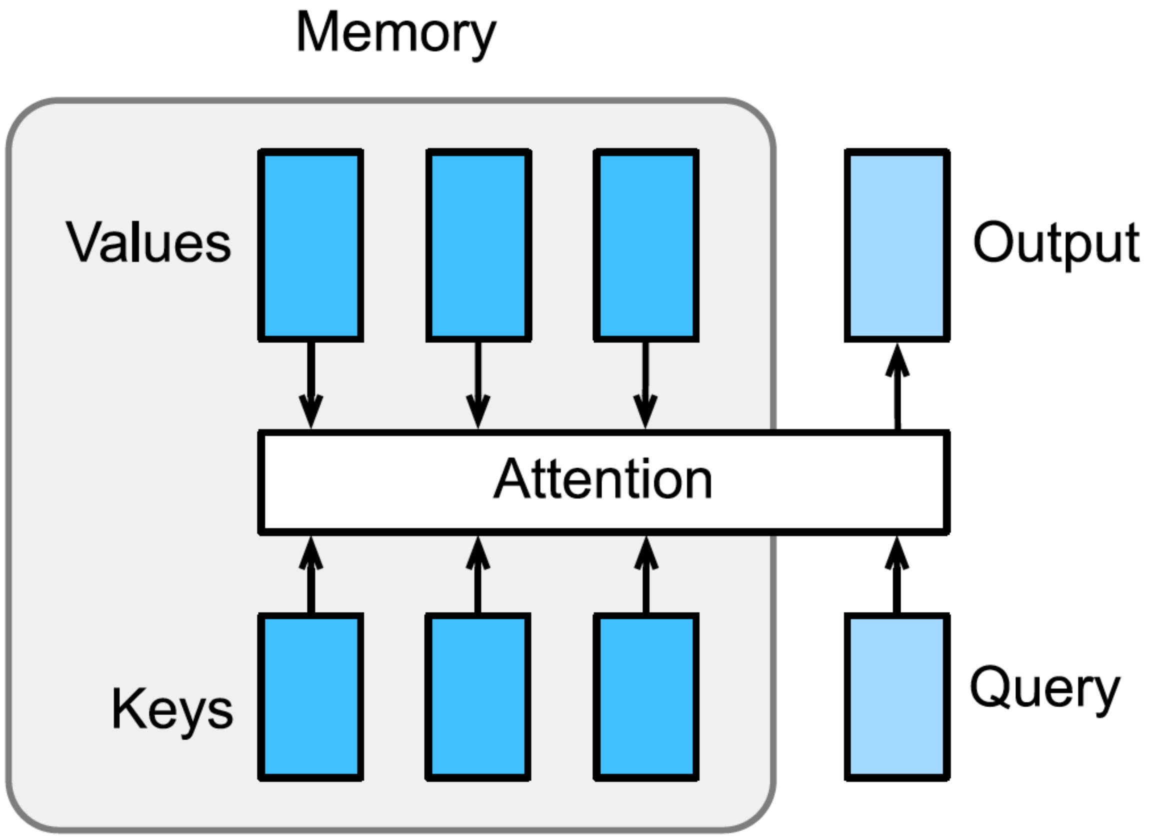

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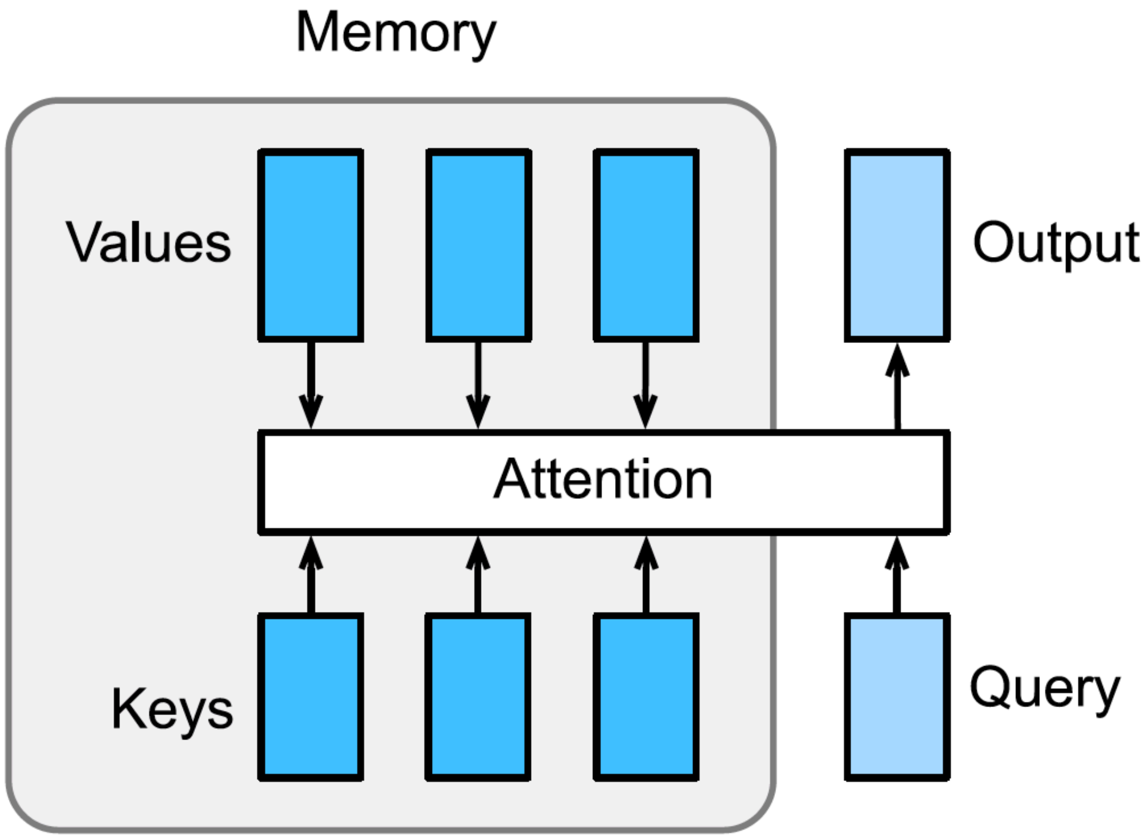

- Assume a query $\mathbf{q} \in \mathbb{R}^{d_q}$
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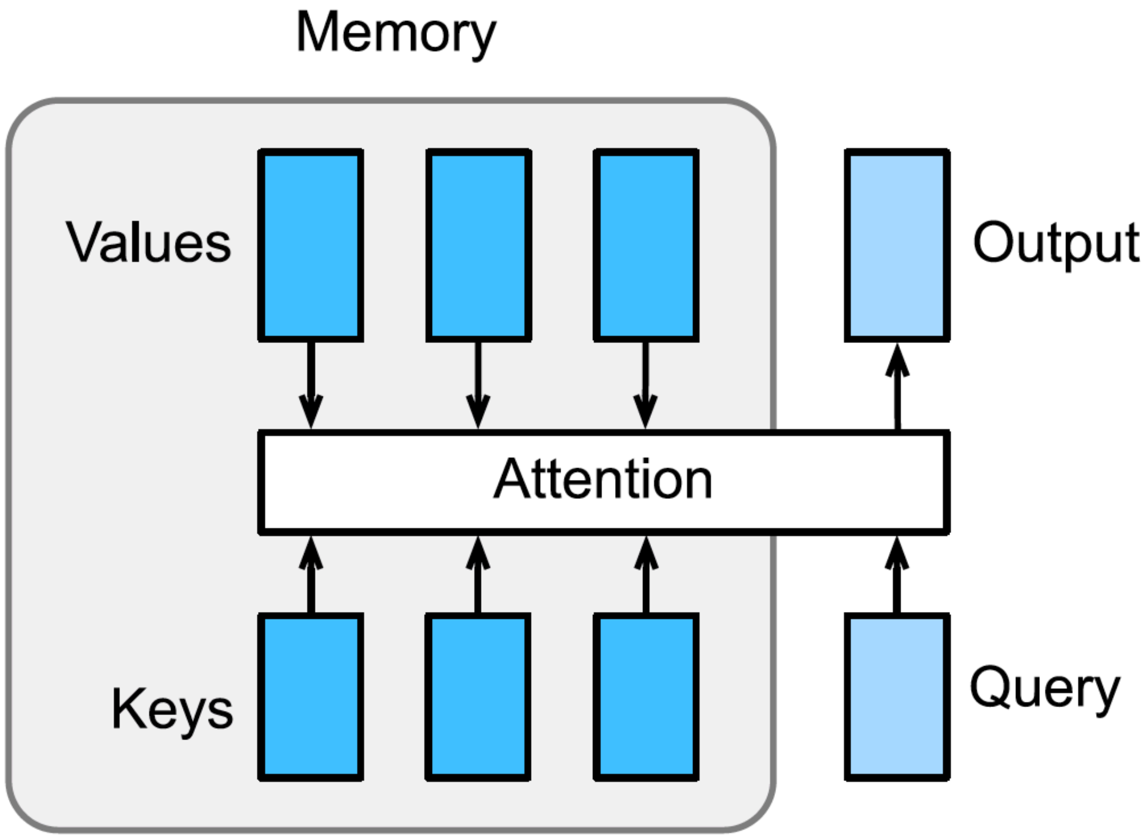

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- The attention layer then returns an output $\mathbf{o} \in \mathbb{R}^{d_v}$

Attention Mechanism

- To compute the output, we first assume there is a score function α which measures the similarity between the query and a key. Then we compute all n scores $a_1, \ldots, a_n$ by

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- Different choices of the score function lead to different attention layers.

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- Assume $\mathbf{Q} \in \mathbb{R}^{m \times d}$ contains m queries and $\mathbf{K} \in \mathbb{R}^{n \times d}$ has all n keys. We can compute all mn scores by

$$\alpha(\mathbf{Q}, \mathbf{K}) = \mathbf{Q}\mathbf{K}^T / \sqrt{d}.$$

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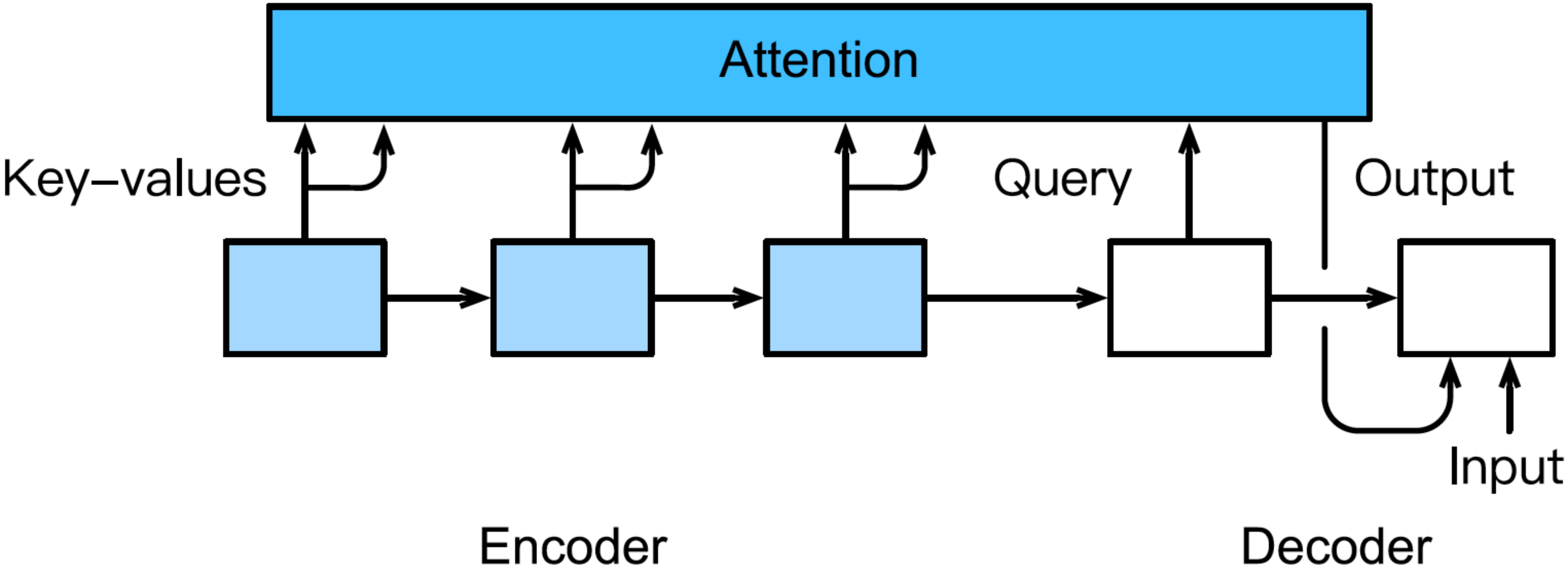
- Given learnable parameters $\mathbf{W}_k \in \mathbb{R}^{h \times d_k}$, $\mathbf{W}_q \in \mathbb{R}^{h \times d_q}$, and $\mathbf{v} \in \mathbb{R}^p$, the score function is defined by

$$\alpha(\mathbf{k}, \mathbf{q}) = \mathbf{v}^T \tanh(\mathbf{W}_k \mathbf{k} + \mathbf{W}_q \mathbf{q}).$$

Sequence to Sequence with Attention Mechanism

- Now, we add the attention mechanism to the sequence to sequence model.



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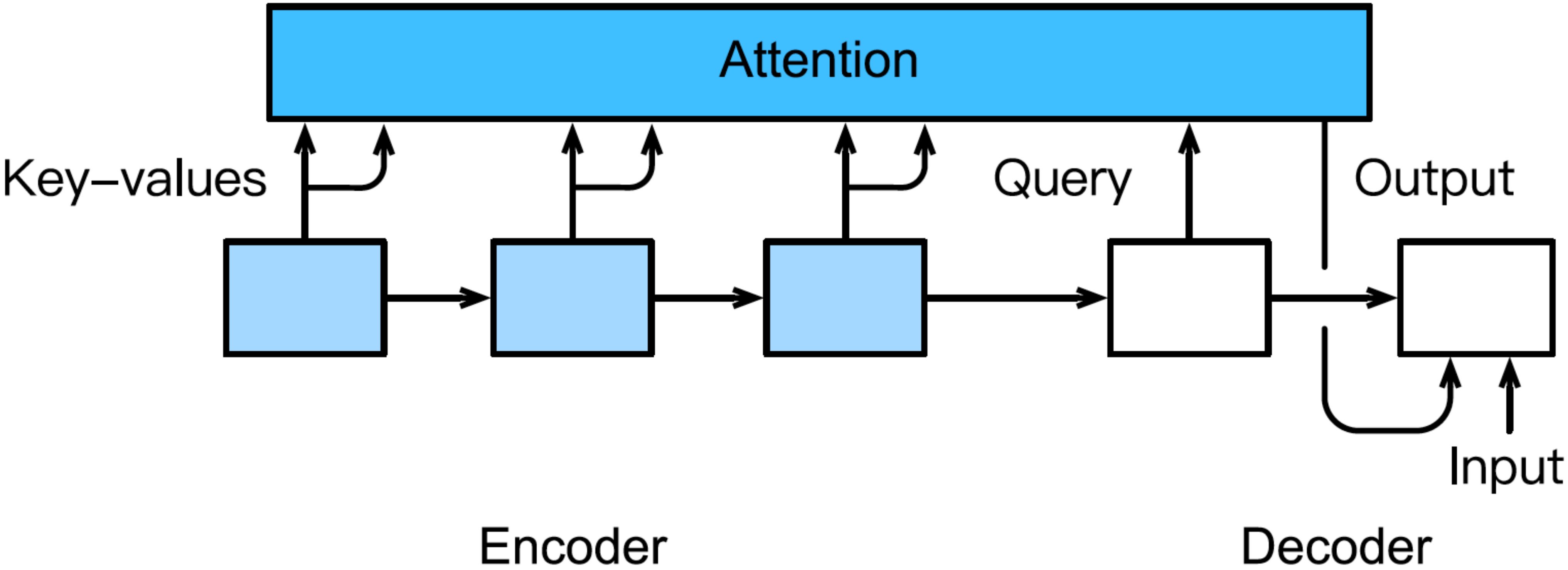

Sequence to Sequence with Attention Mechanism

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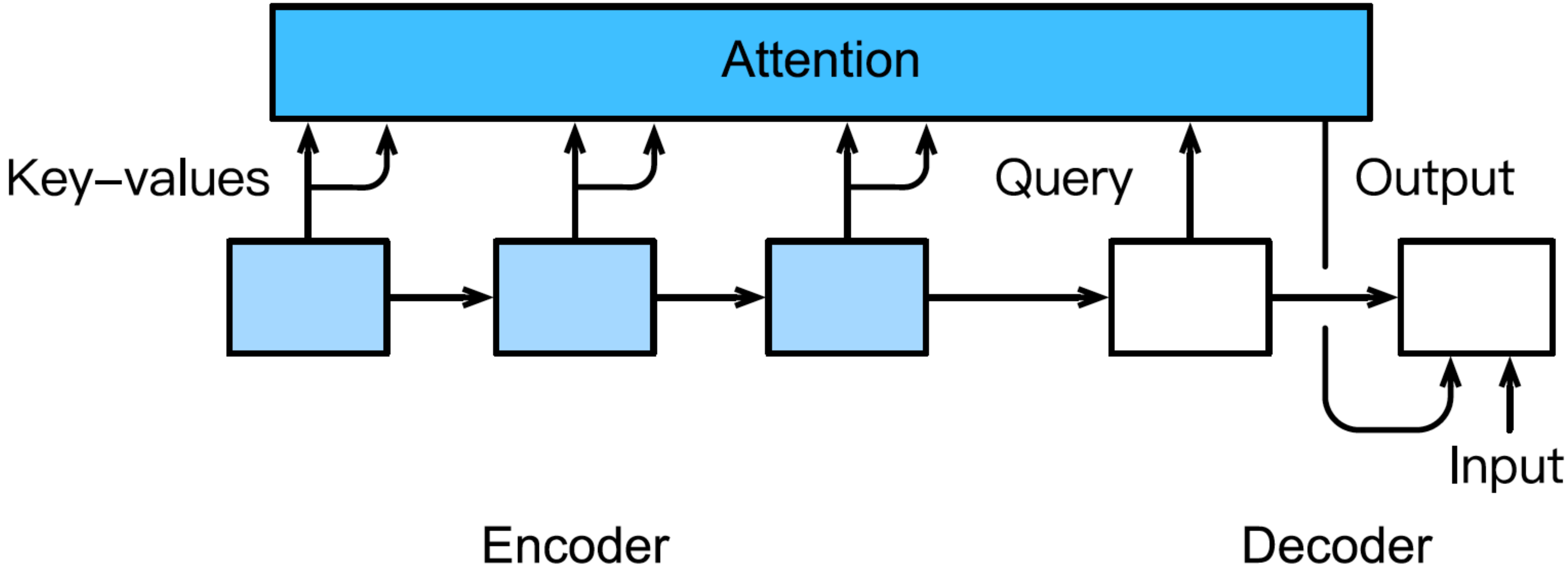
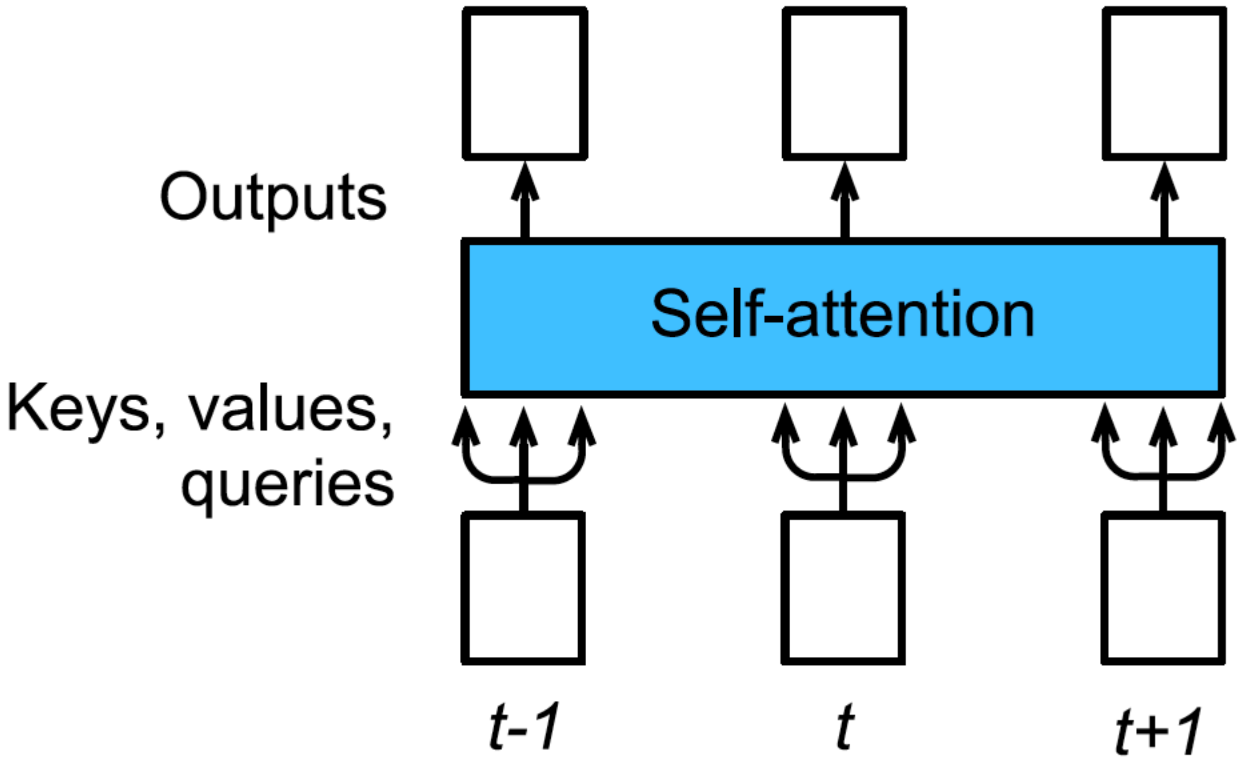
- During decoding, the decoder output from the previous time step is used as the query, the attention output is then fed into the decoder.



Transformer

- The Transformer model is also based on the encoder-decoder architecture.
- The transformer replaces the recurrent layers in seq2seq with attention layers.
- Each item in the sequential is copied as the query, the key and the value.
- We call such an attention layer as a self-attention layer.



Transformer

- The source sequence embeddings are fed into n repeated blocks.
- The outputs of the last block are then used as attention memory for the decoder.
- The target sequence embeddings are similarly fed into n repeated blocks in the decoder.
- The final outputs are obtained by applying a dense layer with vocabulary size to the last block's outputs.