Transformer Model

Shusen Wang

Transformer Model

- **Original paper:** Vaswani et al. Attention Is All You Need. In *NIPS*, 2017.

Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

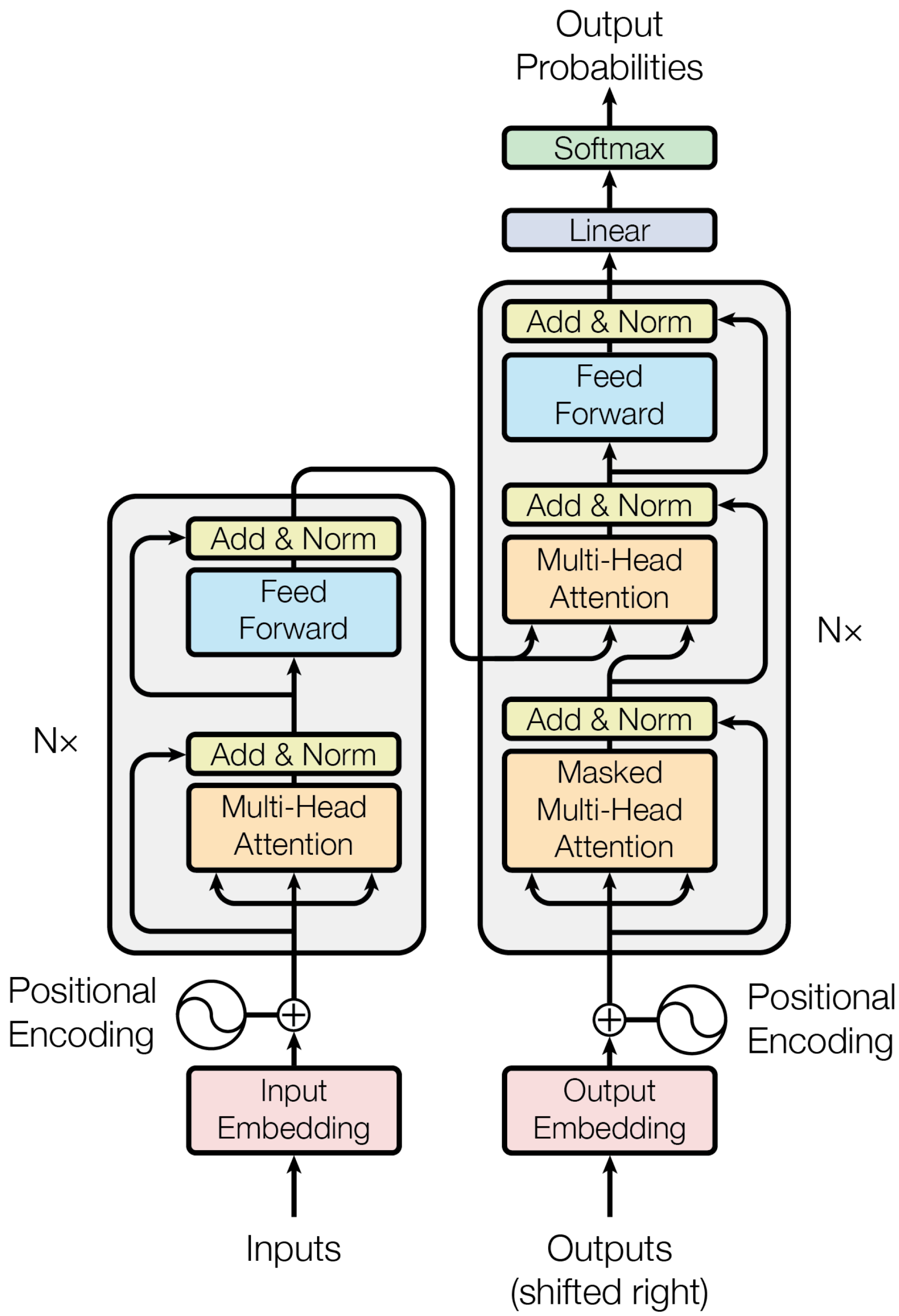
Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

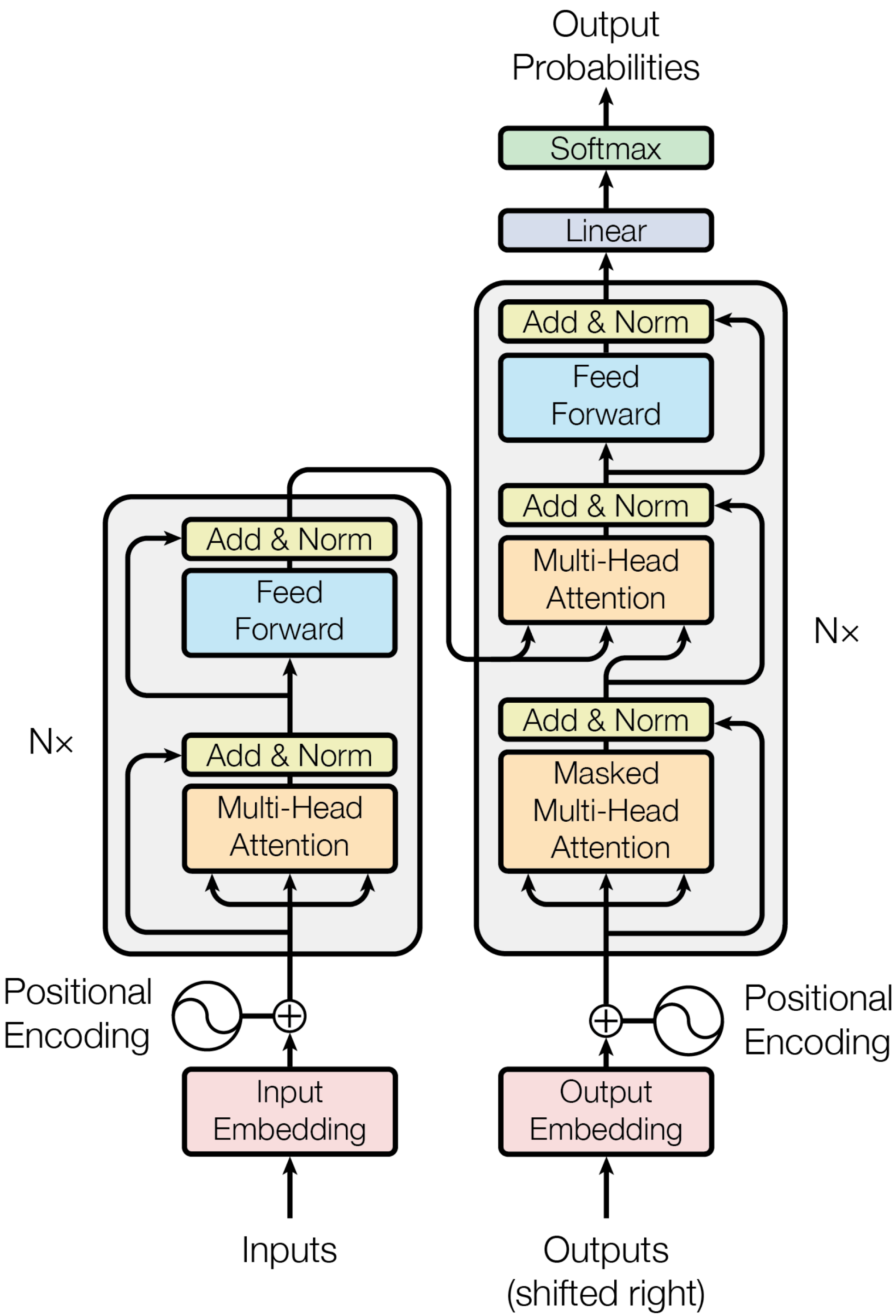
Illia Polosukhin* ‡ illia.polosukhin@gmail.com



Transformer Model

- Transformer is a Seq2Seq model.
- Transformer is not RNN.
- Purely based attention and fully-connected layers.

- Much more computations than RNNs.
- Higher performance than RNNs on large datasets.

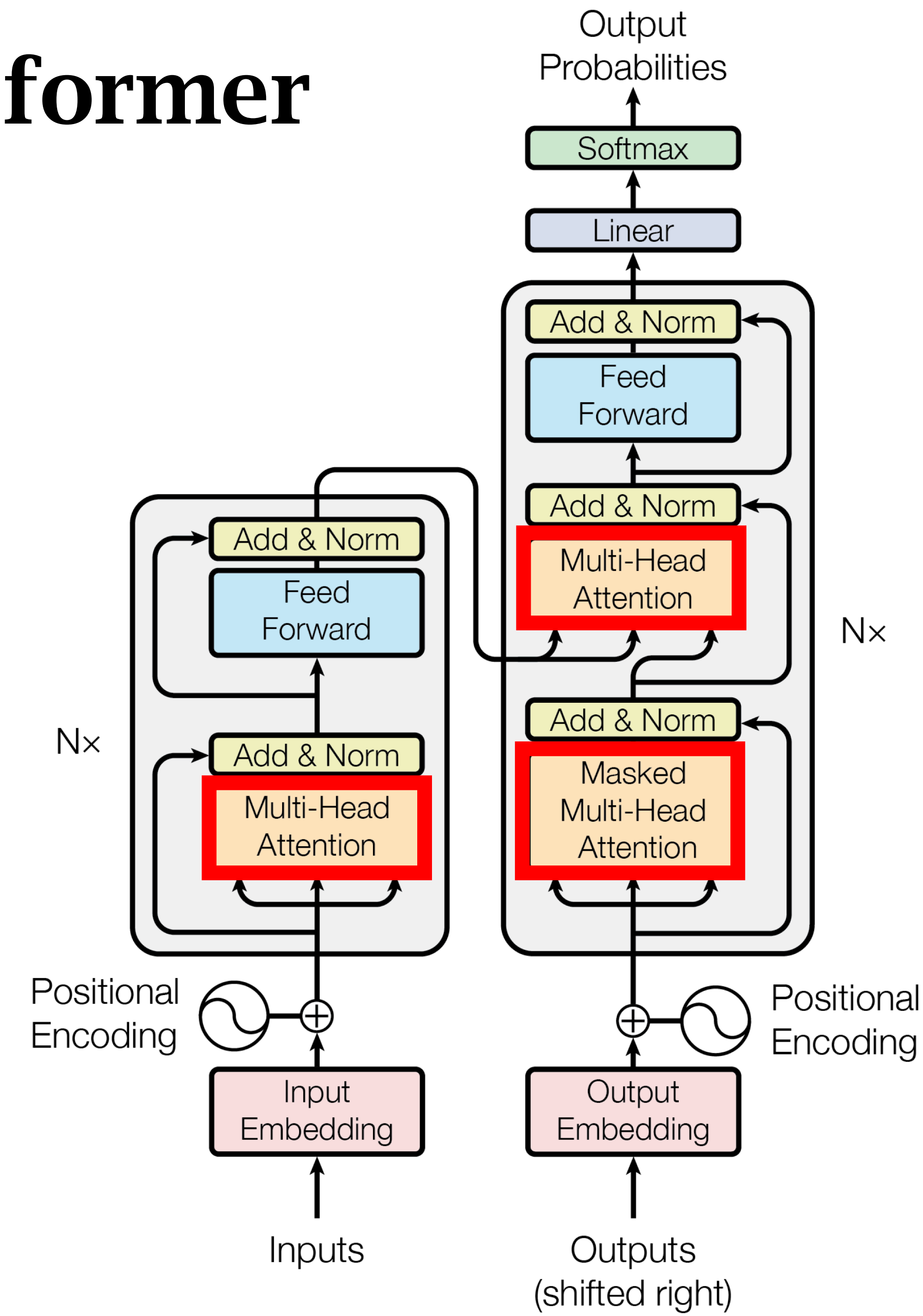


Attention beyond RNNs

Attention in Transformer

Multi-head attention:

- Multiple single-head attentions, each has its own parameter matrices.
- Concatenate the outputs.



Attention in Transformer

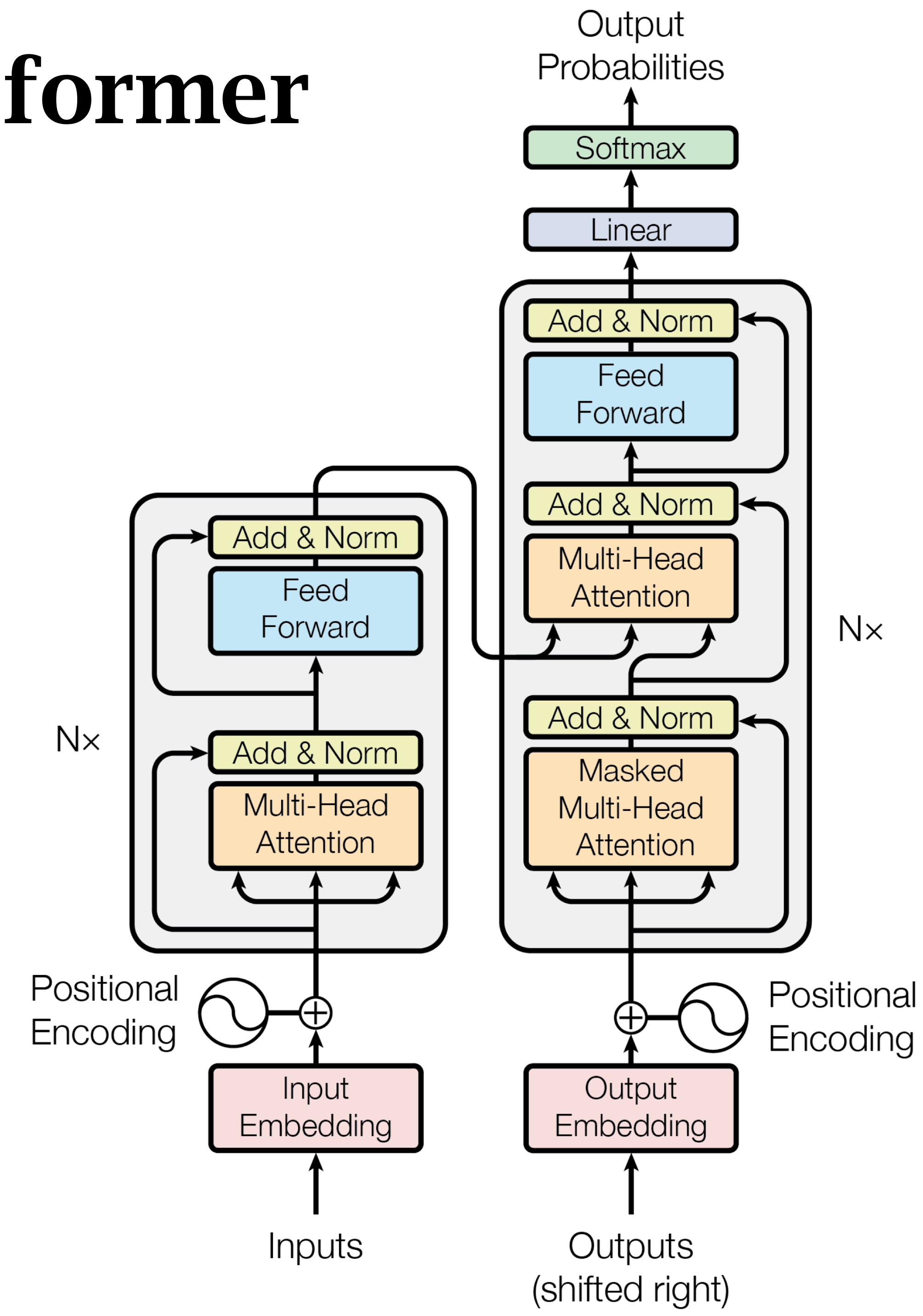
Multi-head attention:

- Multiple single-head attentions, each has its own parameter matrices.
- Concatenate the outputs.

Single-head attention:

- $\mathbf{C} = \text{Attn}(\mathbf{Q},\ \mathbf{K},\ \mathbf{V})$.

query key value



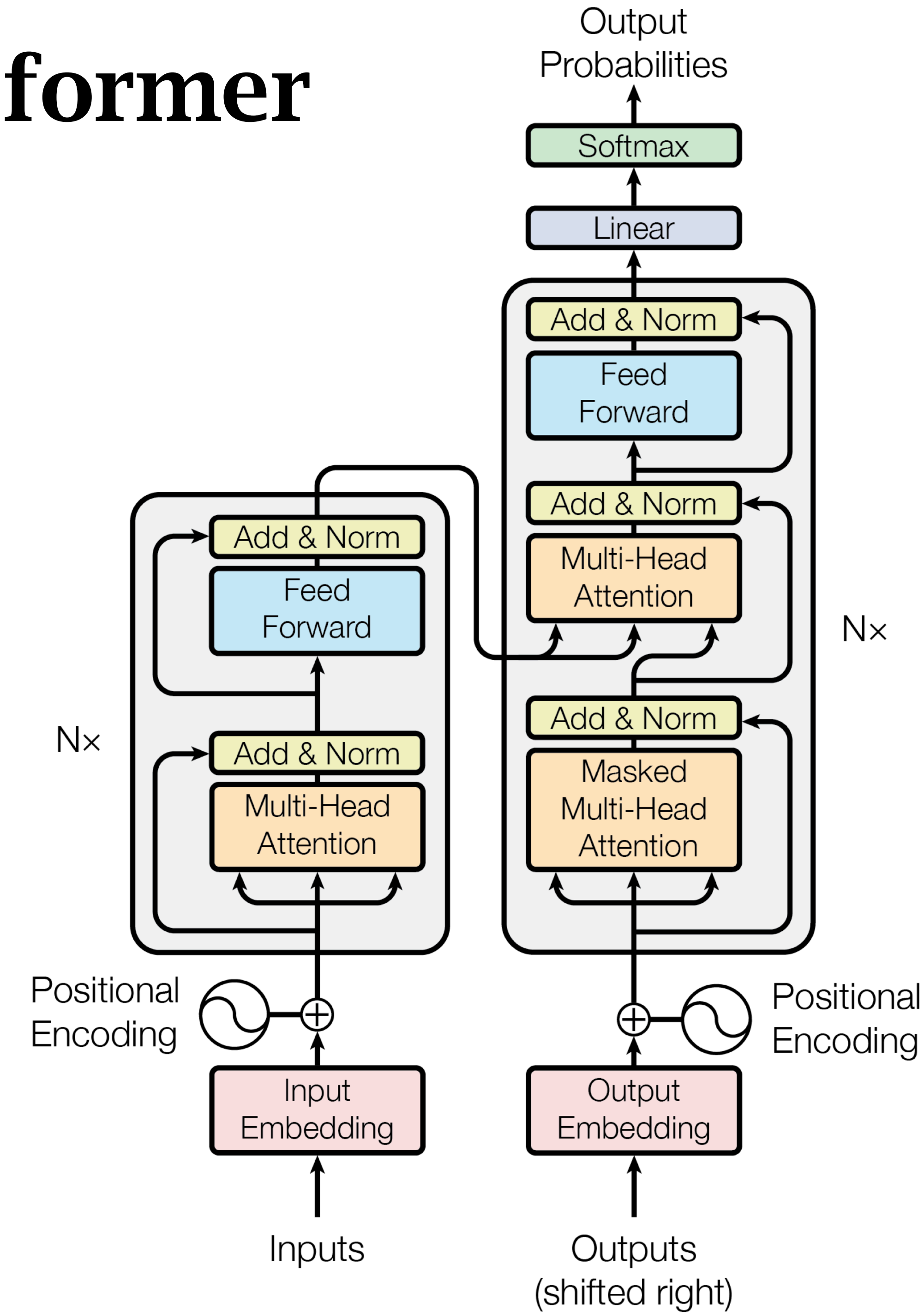
Attention in Transformer

Multi-head attention:

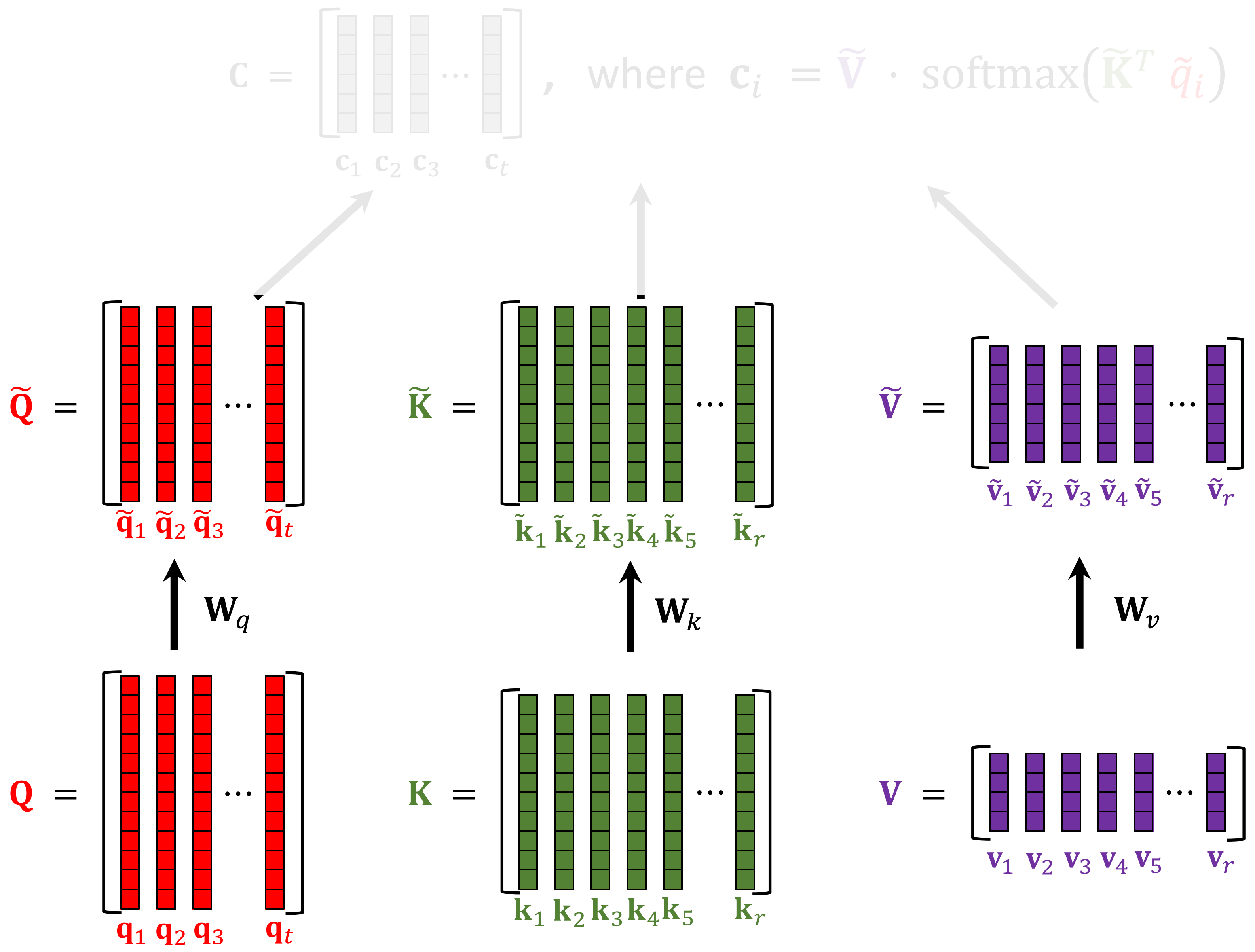
- Multiple single-head attentions, each has its own parameter matrices.
- Concatenate the outputs.

Single-head attention:

- $\mathbf{C} = \mathrm{Attn}(\mathbf{Q},\ \mathbf{K},\ \mathbf{V})$.
- $\mathbf{Q}$ and $\mathbf{C}$ have t columns.
- t: sequence length.
- $\mathbf{K}$ and $\mathbf{V}$ have r columns (r is arbitrary).



Single-Head Attention: $\mathbf{C} = \mathrm{Attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V})$.



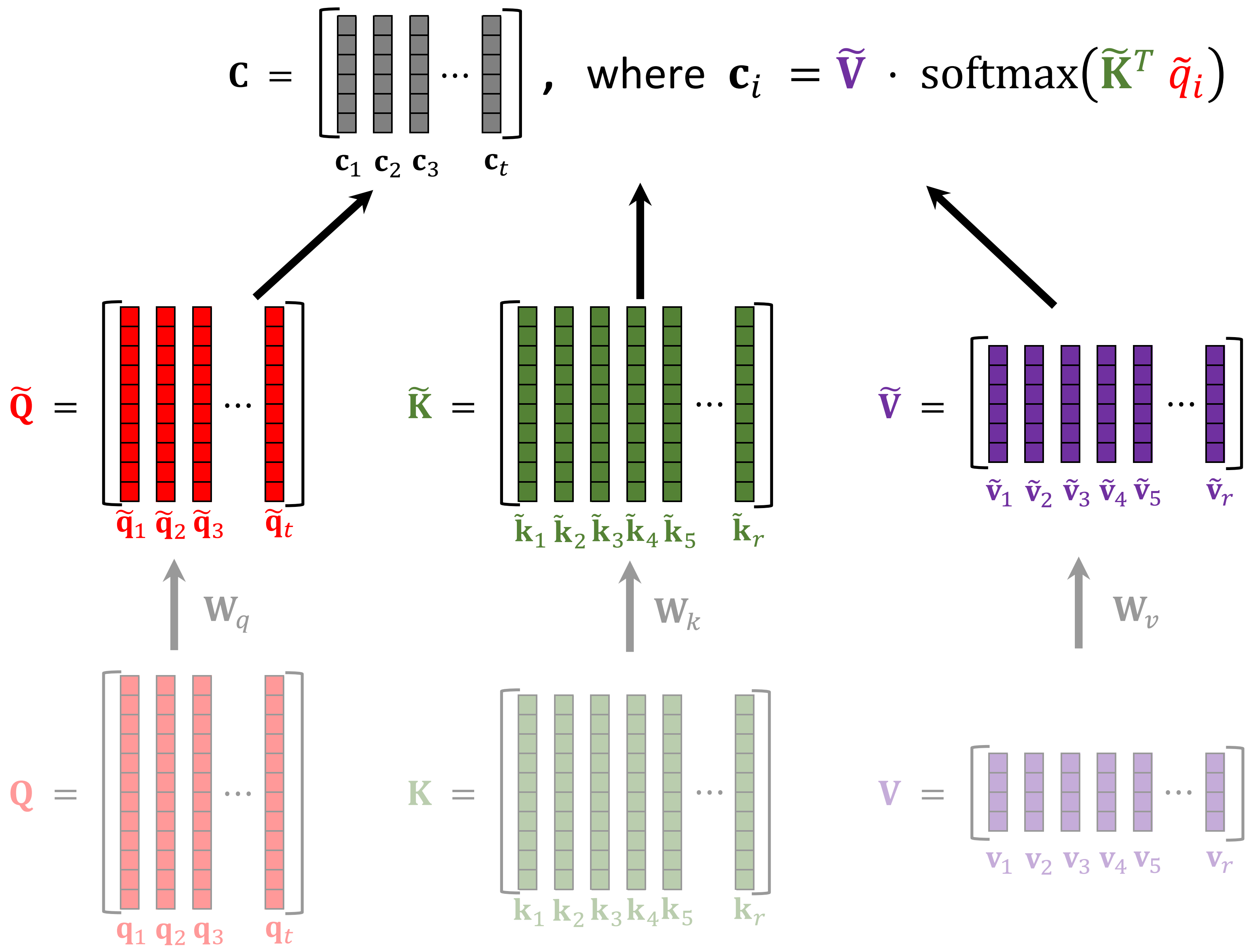
Linear maps:

- $\tilde{\mathbf{Q}} = \mathbf{W}_q \mathbf{Q}$,
- $\tilde{\mathbf{K}} = \mathbf{W}_k \mathbf{K}$,
- $\tilde{\mathbf{V}} = \mathbf{W}_v \mathbf{V}$.

Trainable parameters:

- $\mathbf{W}_q, \mathbf{W}_k, \mathbf{W}_v$.

Single-Head Attention: $\mathbf{C} = \mathrm{Attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V})$.



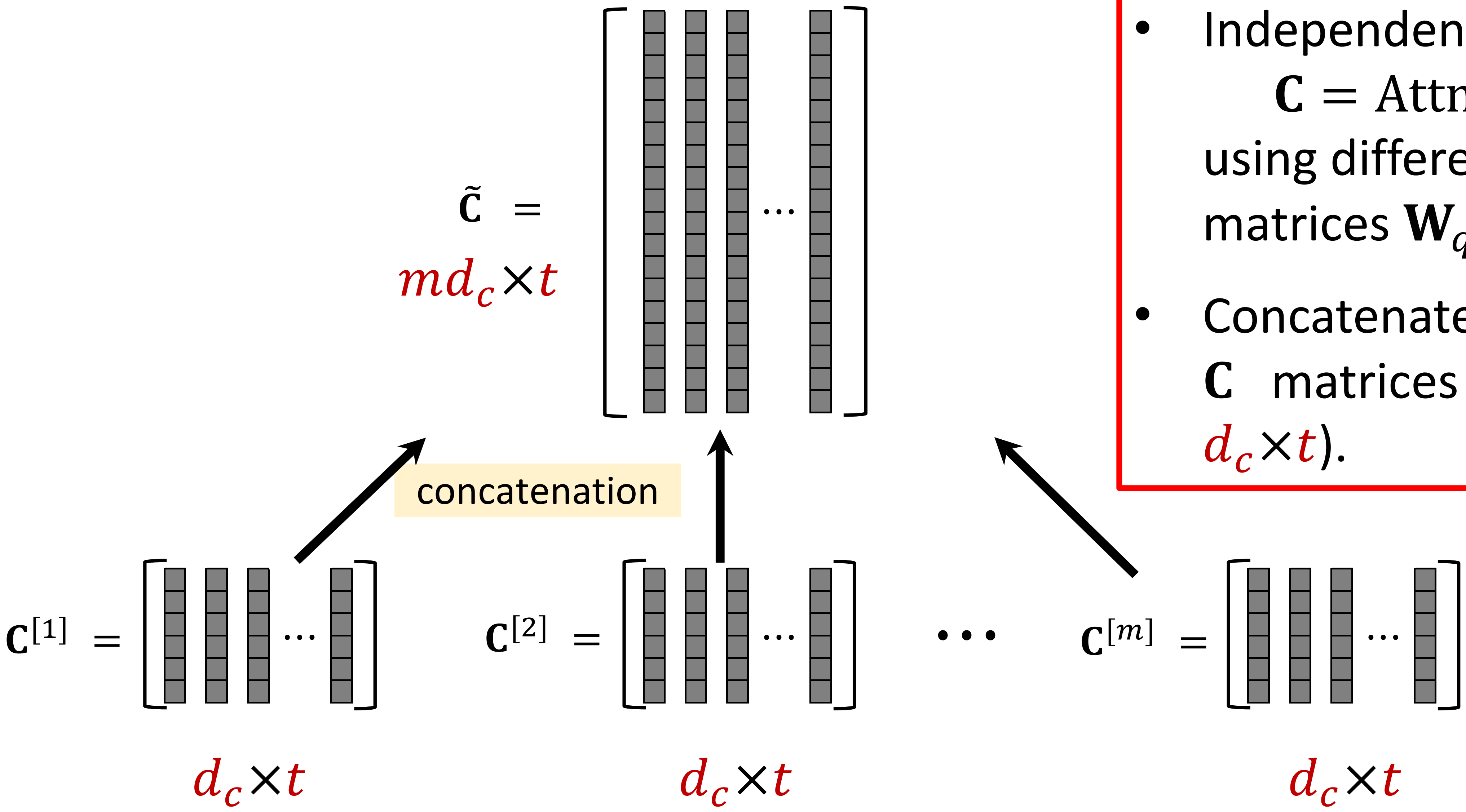
Single-Head Attention: $\mathbf{C} = \mathrm{Attn}(\mathbf{Q},\ \mathbf{K},\ \mathbf{V})$.

$$\mathbf{C} = \begin{bmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \mathbf{c}_3 & \cdots & \mathbf{c}_t \end{bmatrix}, \quad \text{where} \quad \boxed{\mathbf{c}_i = \tilde{\mathbf{V}} \cdot \mathrm{softmax}(\tilde{\mathbf{K}}^T \tilde{q}_i)}$$

For i from 1 to t:

- Weights: $\tilde{\boldsymbol{\alpha}} = \tilde{\mathbf{K}}^T \cdot \tilde{\mathbf{q}}_i \in \mathbb{R}^r$.
  - $\tilde{\alpha}_p = \mathrm{similarity}(\tilde{\mathbf{k}}_p,\ \tilde{\mathbf{q}}_i)$.
  - Here, it uses inner product to measure similarity.
- Normalized weights: $\boldsymbol{\alpha} = \mathrm{Softmax}(\tilde{\boldsymbol{\alpha}})$.
- Context vector: $\mathbf{c}_i = \tilde{\mathbf{V}} \cdot \boldsymbol{\alpha} = \alpha_1 \tilde{\mathbf{v}}_1 + \cdots + \alpha_r \tilde{\mathbf{v}}_r$.

Multi-Head Attention

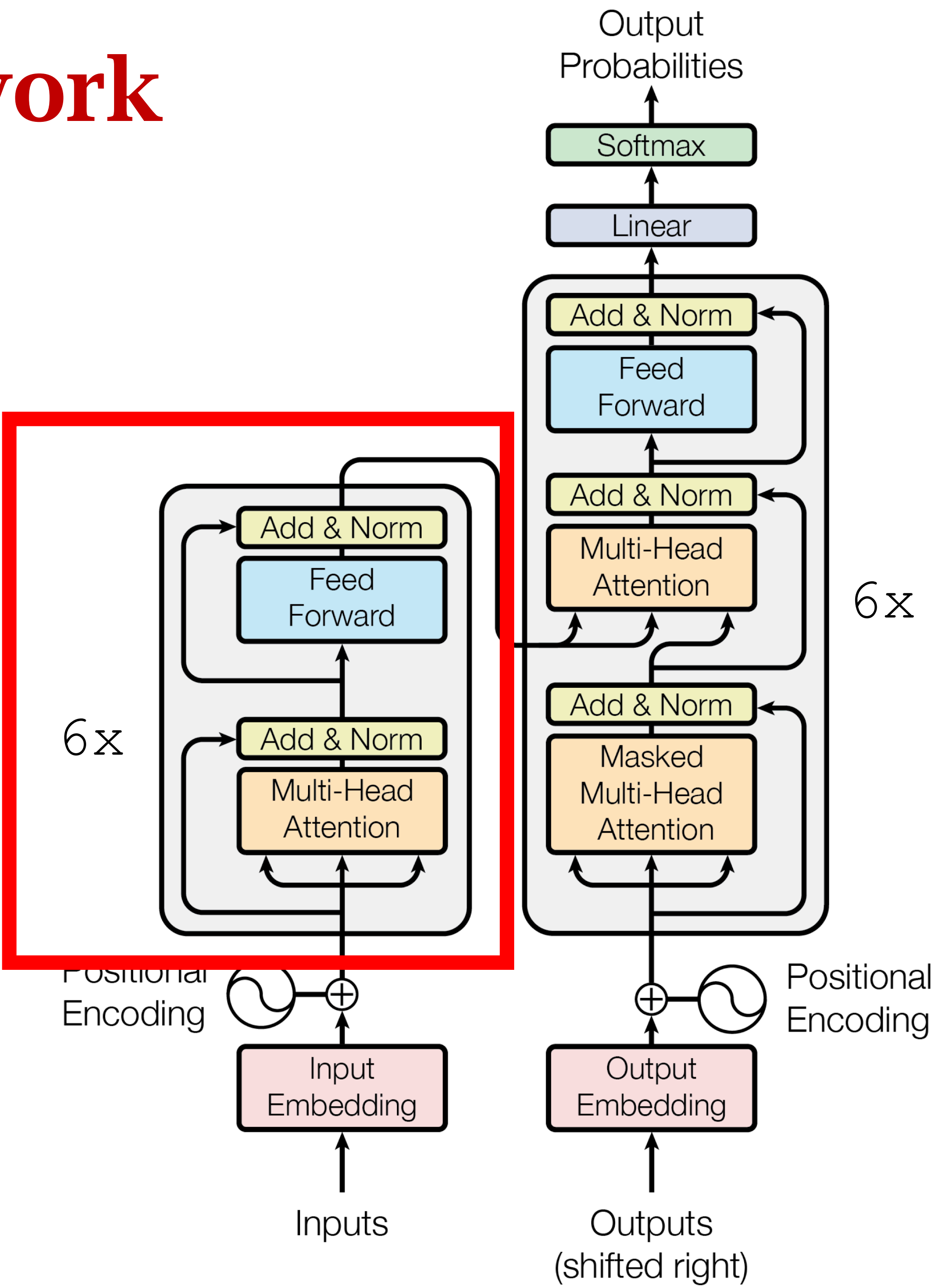


- Independently perform
  $$\mathbf{C} = \mathrm{Attn}(\mathbf{Q}, \ \mathbf{K}, \ \mathbf{V})$$
  using different parameter matrices $\mathbf{W}_q$, $\mathbf{W}_k$, and $\mathbf{W}_v$.
- Concatenate the obtained $\mathbf{C}$ matrices (which are $d_c \times t$).

Encoder of Transformer

Encoder Network

- Encoder has 6 blocks.
- 1 Block = Multi-head attention + Dense.
- 6 is the result of hyper-parameter tuning; nothing magical about 6.
- Other tricks:
  - Skip connection.
  - Normalization.



Multi-Head Attention + Dense Layer

Multi-Head Attention

$$\tilde{\mathbf{C}} = [\ \tilde{\mathbf{c}}_1,\ \tilde{\mathbf{c}}_2,\ \tilde{\mathbf{c}}_3, \cdots,\ \tilde{\mathbf{c}}_t\ ] \in \mathbb{R}^{md_c \times t}$$

Concatenation

$$\mathbf{C}^{[1]} \in \mathbb{R}^{d_c \times t} \qquad \mathbf{C}^{[2]} \in \mathbb{R}^{d_c \times t} \qquad \cdots \qquad \mathbf{C}^{[m]} \in \mathbb{R}^{d_c \times t}$$

Attention w/ different parameter matrices.

$$(\mathbf{Q},\ \mathbf{K},\ \mathbf{V})$$

Multi-Head Attention + Dense Layer

$\tilde{\mathbf{C}}$'s number of columns, t, is determined by **Q**.

Multi-Head Attention

$$\tilde{\mathbf{C}} = [\, \tilde{\mathbf{c}}_1, \quad \tilde{\mathbf{c}}_2, \quad \tilde{\mathbf{c}}_3, \cdots, \quad \tilde{\mathbf{c}}_t \,] \in \mathbb{R}^{md_c \times t}$$

Concatenation

$$\mathbf{C}^{[1]} \in \mathbb{R}^{d_c \times t} \qquad \mathbf{C}^{[2]} \in \mathbb{R}^{d_c \times t} \qquad \cdots \qquad \mathbf{C}^{[m]} \in \mathbb{R}^{d_c \times t}$$

Attention w/ different parameter matrices.

$$(\mathbf{Q}, \quad \mathbf{K}, \quad \mathbf{V})$$

Multi-Head Attention + Dense Layer

$$\tilde{\mathbf{U}} = [\ \tilde{\mathbf{u}}_1,\ \tilde{\mathbf{u}}_2,\ \tilde{\mathbf{u}}_3, \cdots,\ \tilde{\mathbf{u}}_t\ ] \in \mathbb{R}^{d_u \times t}$$

Dense layer is applied to every column independently.

$\cdots$

$$\tilde{\mathbf{C}} = [\ \tilde{\mathbf{c}}_1,\ \tilde{\mathbf{c}}_2,\ \tilde{\mathbf{c}}_3, \cdots,\ \tilde{\mathbf{c}}_t\ ] \in \mathbb{R}^{md_c \times t}$$

Concatenation

$\mathbf{C}^{[1]} \in \mathbb{R}^{d_c \times t}$ $\quad$ $\mathbf{C}^{[2]} \in \mathbb{R}^{d_c \times t}$ $\quad \cdots \quad$ $\mathbf{C}^{[m]} \in \mathbb{R}^{d_c \times t}$

Attention w/ different parameter matrices.

$(\mathbf{Q},\quad \mathbf{K},\quad \mathbf{V})$

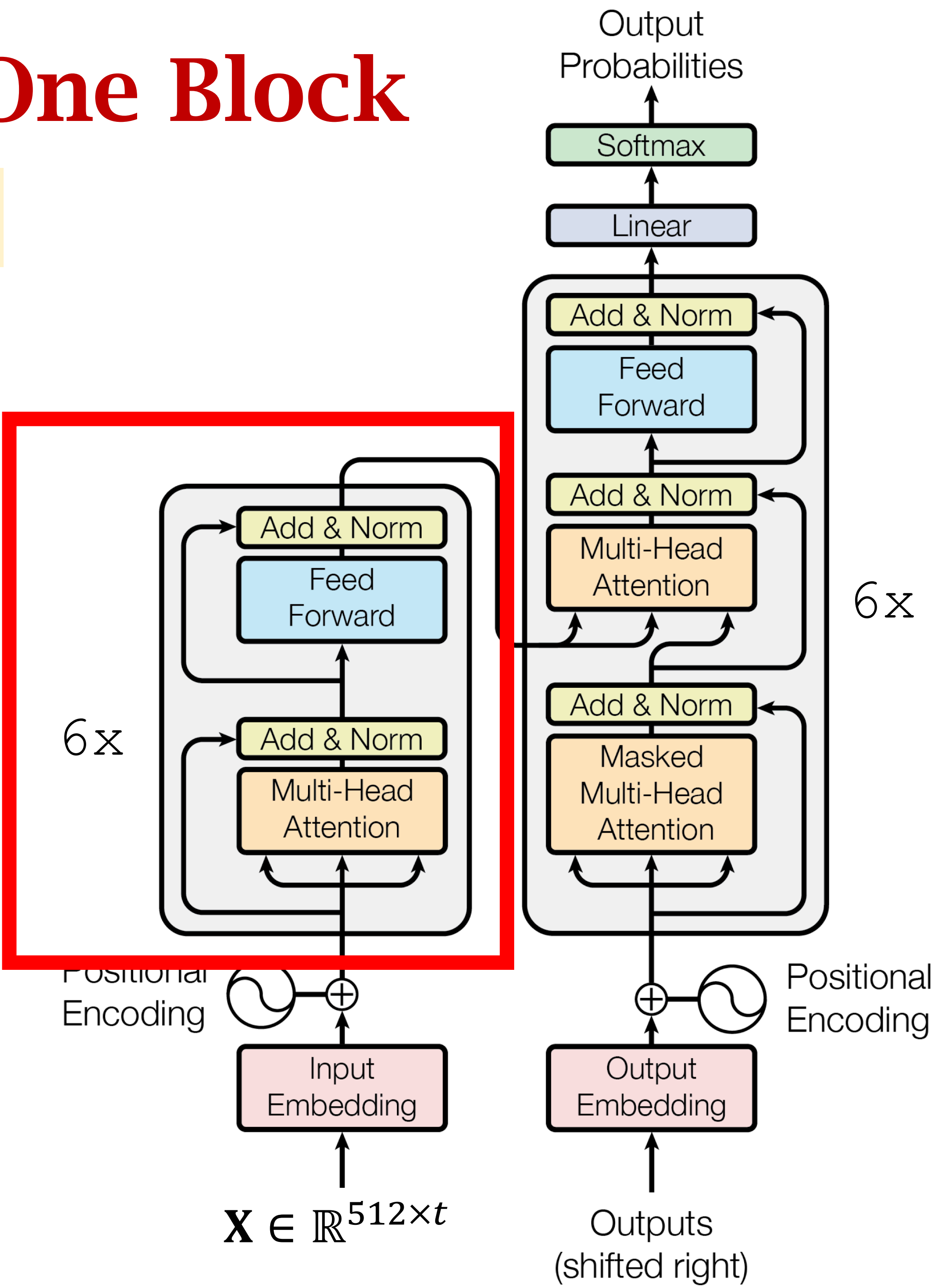
Encoder Network: One Block

Ignore skip connection and normalization.

- Input: $\mathbf{X} \in \mathbb{R}^{512 \times t}$; ($t$ is the seq length.)
- Set $\mathbf{Q} = \mathbf{K} = \mathbf{V} = \mathbf{X}$.

query key value

Similar to self-attention.



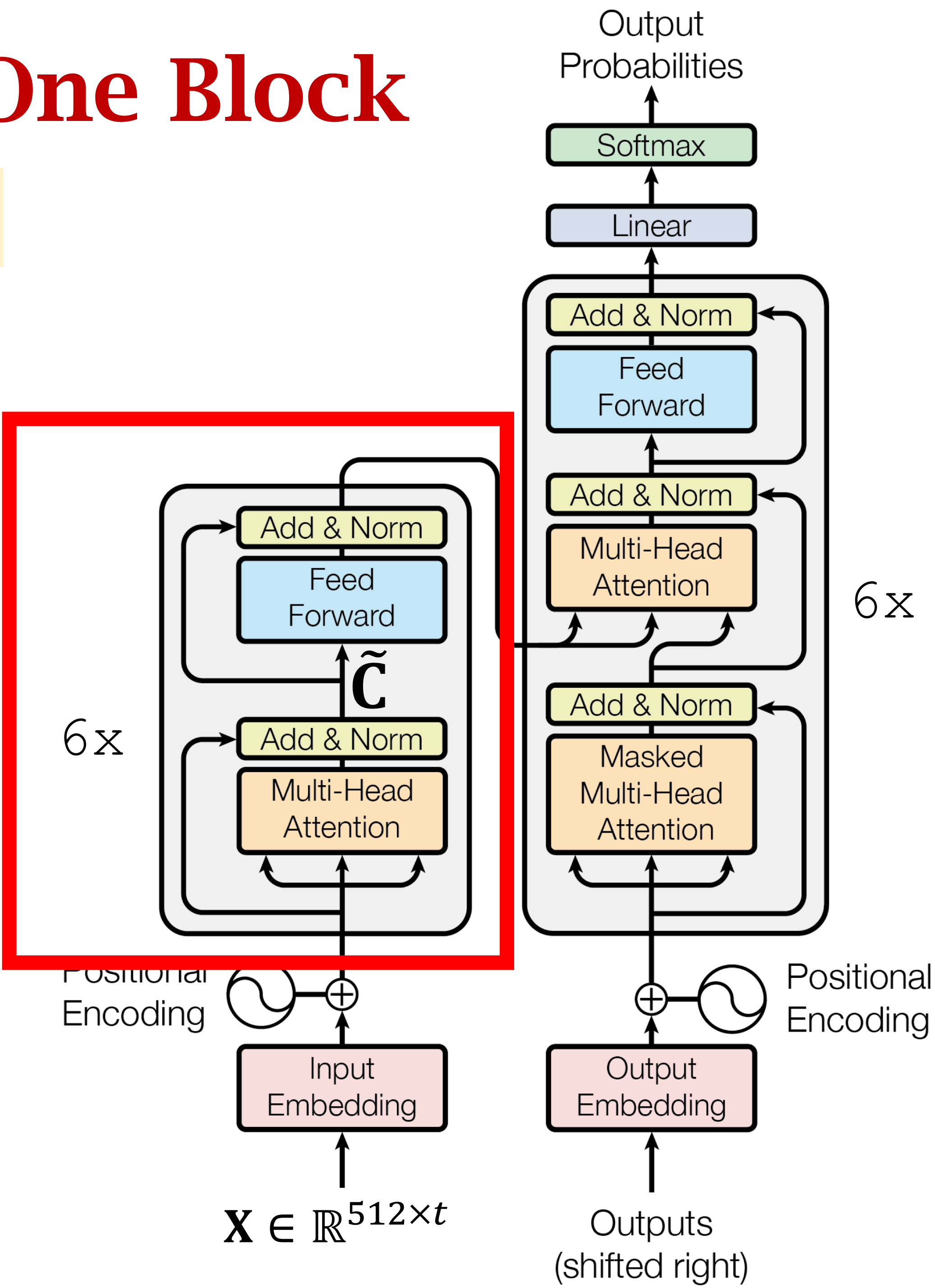
Encoder Network: One Block

Ignore skip connection and normalization.

- Input: $\mathbf{X} \in \mathbb{R}^{512 \times t}$; ($t$ is the seq length.)
- Set $\mathbf{Q} = \mathbf{K} = \mathbf{V} = \mathbf{X}$.
- Repeat $m = 8$ times:

$$\mathbf{C}^{[i]} = \text{Attn}(\mathbf{Q}, \ \mathbf{K}, \ \mathbf{V}) \in \mathbb{R}^{64 \times t}.$$

- $\tilde{\mathbf{C}} = \text{Concatenate}\left(\mathbf{C}^{[1]}, \cdots, \mathbf{C}^{[m]}\right) \in \mathbb{R}^{512 \times t}$.



- Make sure the input shape and output shape are the same.
- Otherwise, skip connection cannot be applied.

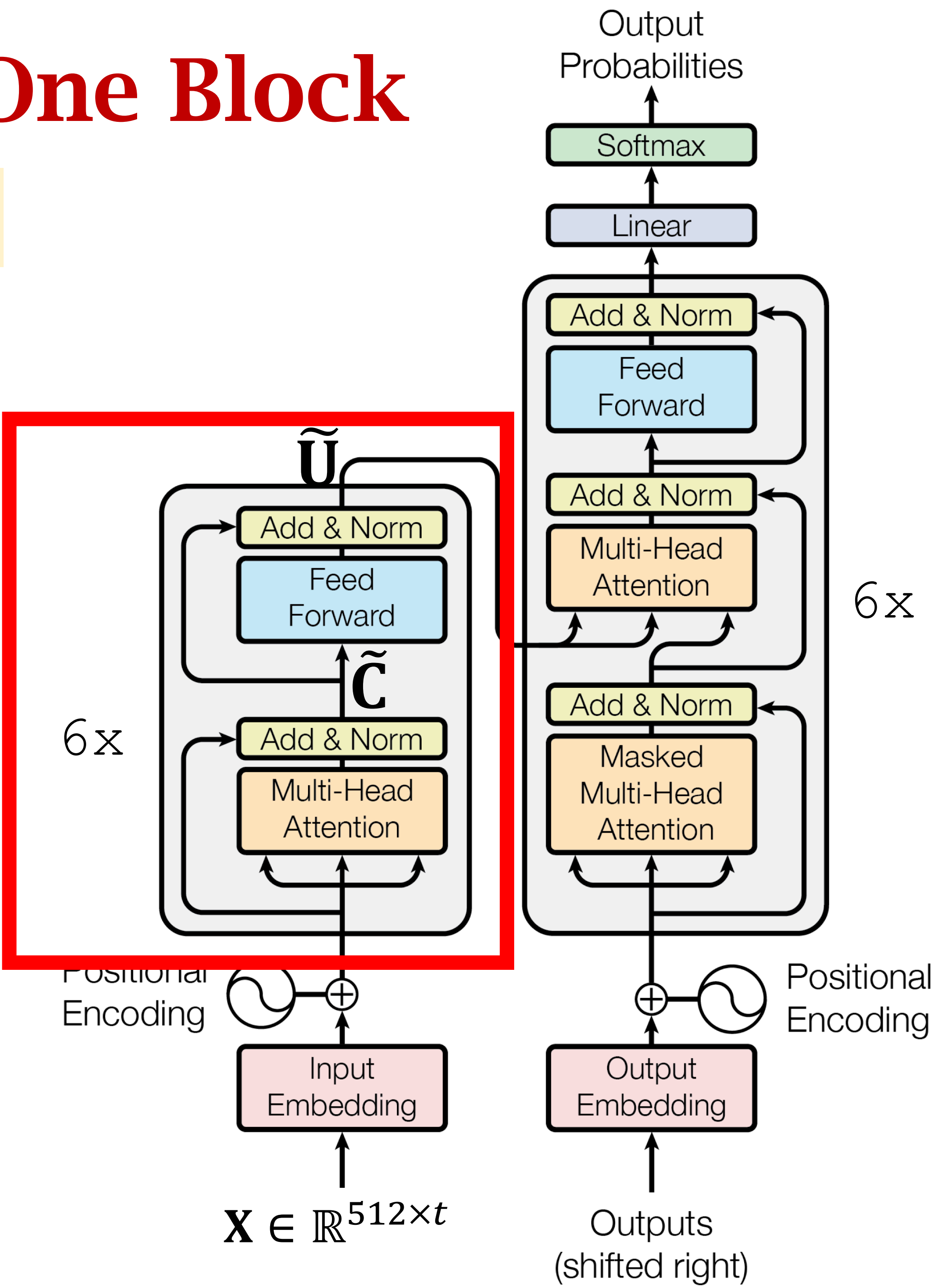
Encoder Network: One Block

Ignore skip connection and normalization.

- Input: $\mathbf{X} \in \mathbb{R}^{512 \times t}$; ($t$ is the seq length.)
- Set $\mathbf{Q} = \mathbf{K} = \mathbf{V} = \mathbf{X}$.
- Repeat $m = 8$ times:

$$\mathbf{C}^{[i]} = \text{Attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) \in \mathbb{R}^{64 \times t}.$$

- $\tilde{\mathbf{C}} = \text{Concatenate}\left(\mathbf{C}^{[1]}, \cdots, \mathbf{C}^{[m]}\right) \in \mathbb{R}^{512 \times t}$.
- $\tilde{\mathbf{U}} = \text{DenseLayer}\left(\tilde{\mathbf{C}}\right) \in \mathbb{R}^{512 \times t}$.
- Output: $\tilde{\mathbf{U}} \in \mathbb{R}^{512 \times t}$. (The same shape as $\mathbf{X}$.)

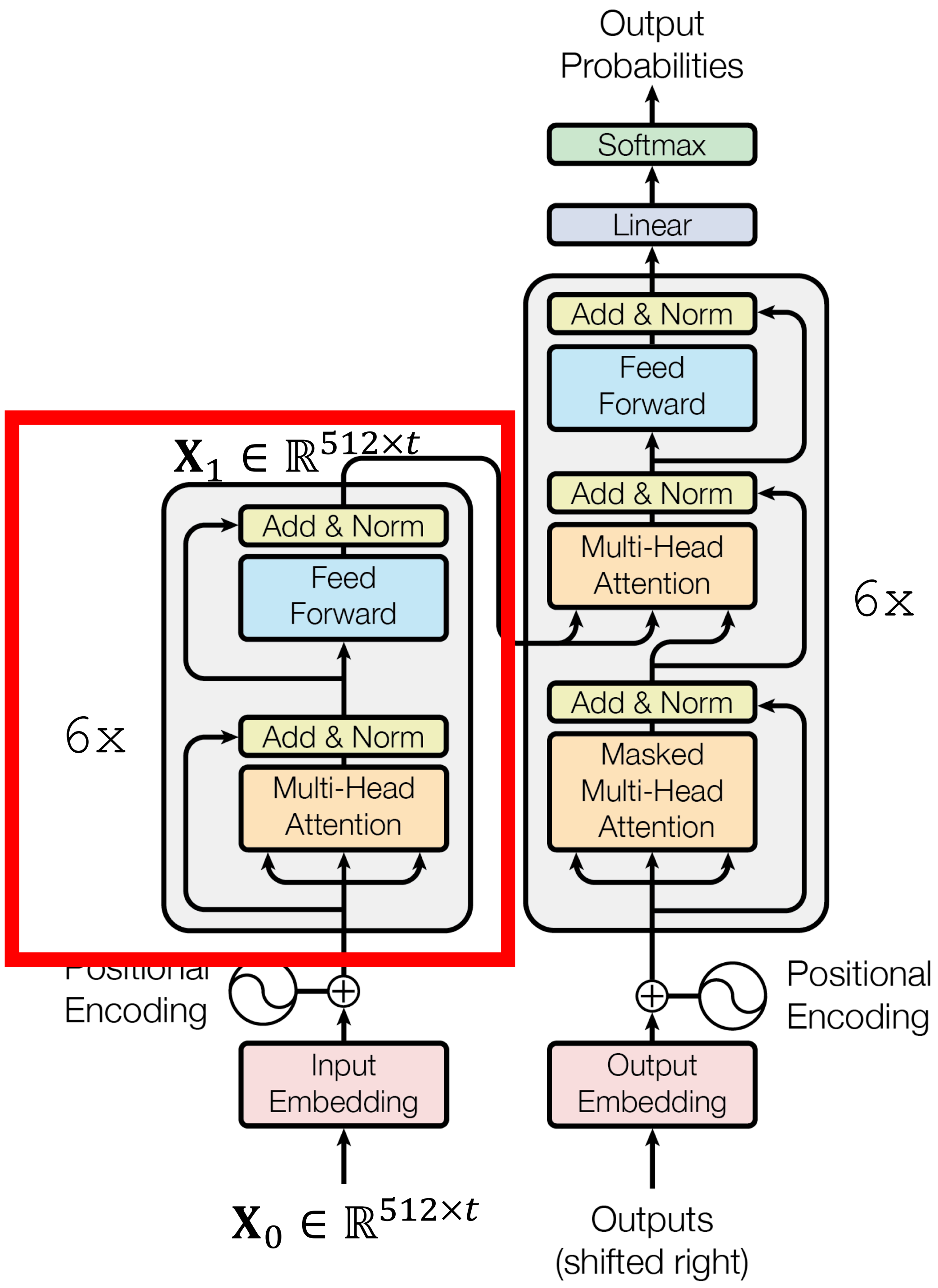


Encoder Network

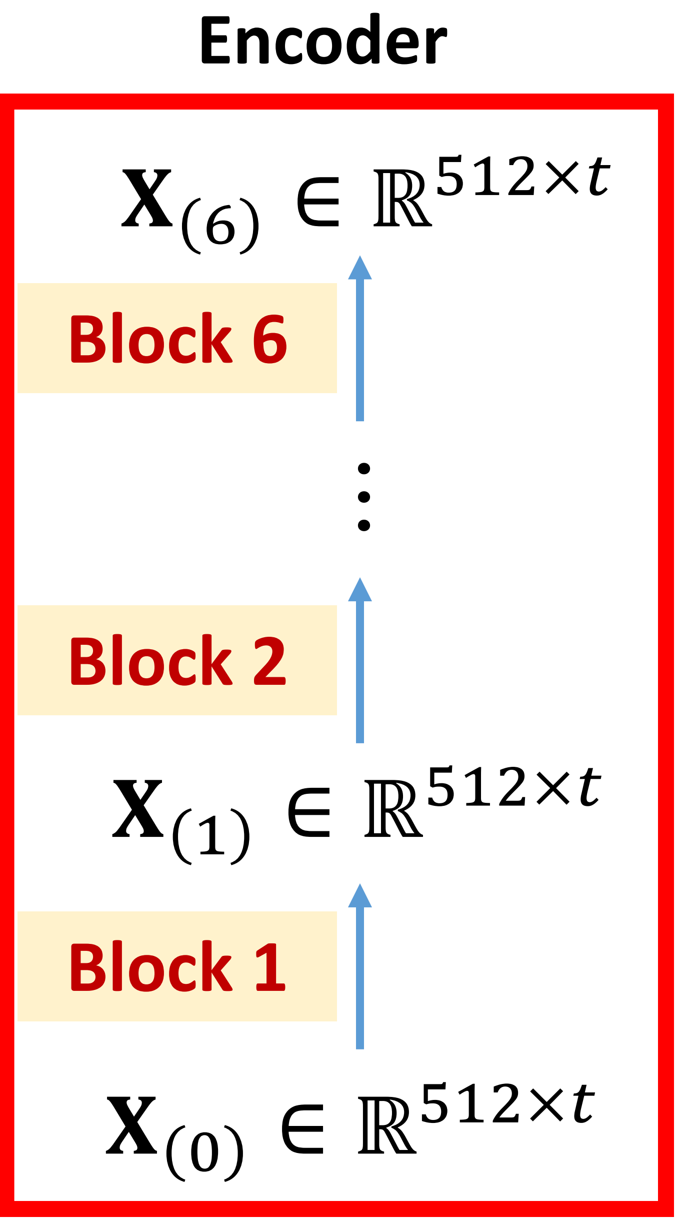
$\mathbf{X}_{(1)} \in \mathbb{R}^{512\times t}$

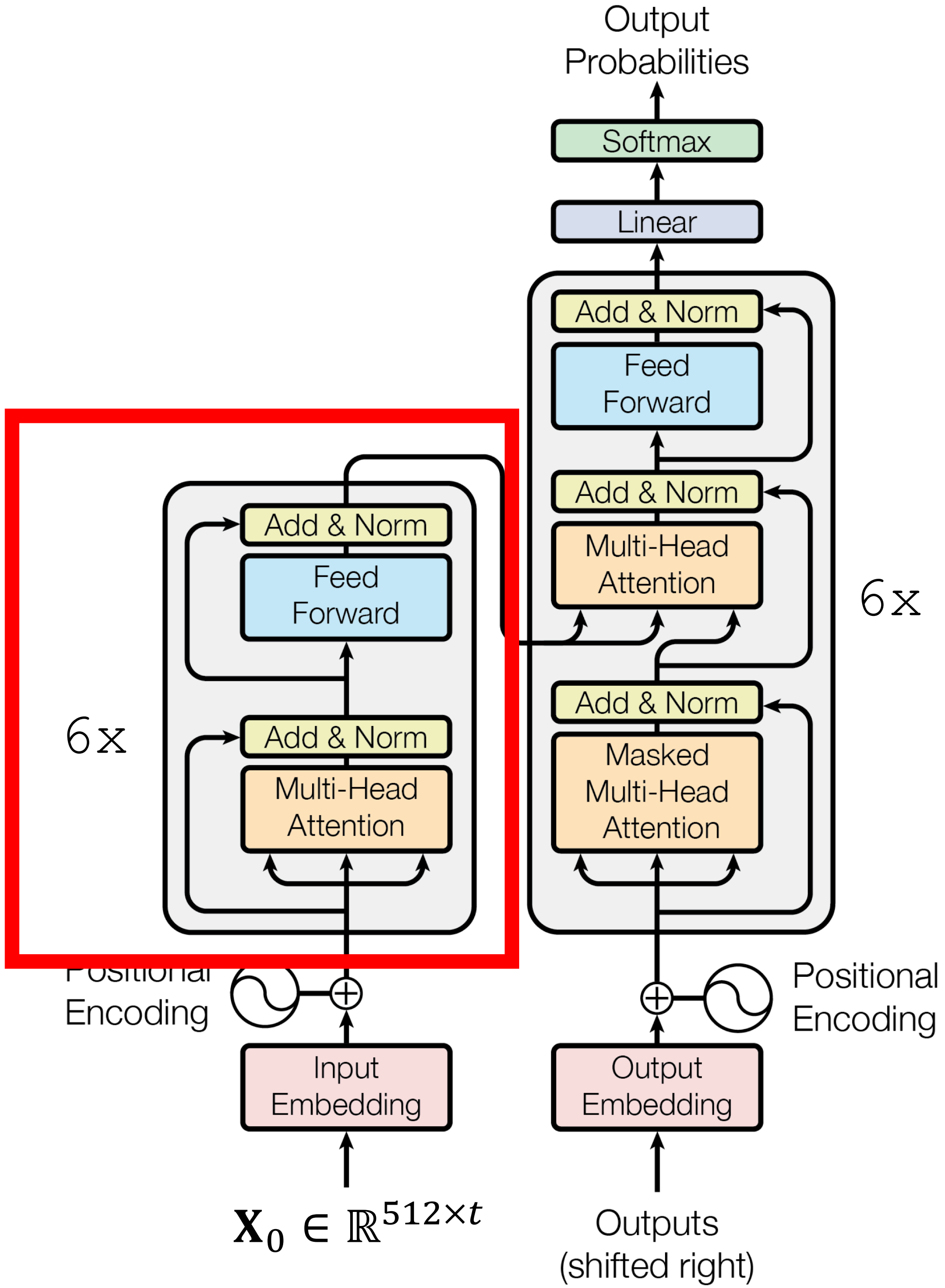
Block 1

$\mathbf{X}_{(0)} \in \mathbb{R}^{512\times t}$



Encoder Network

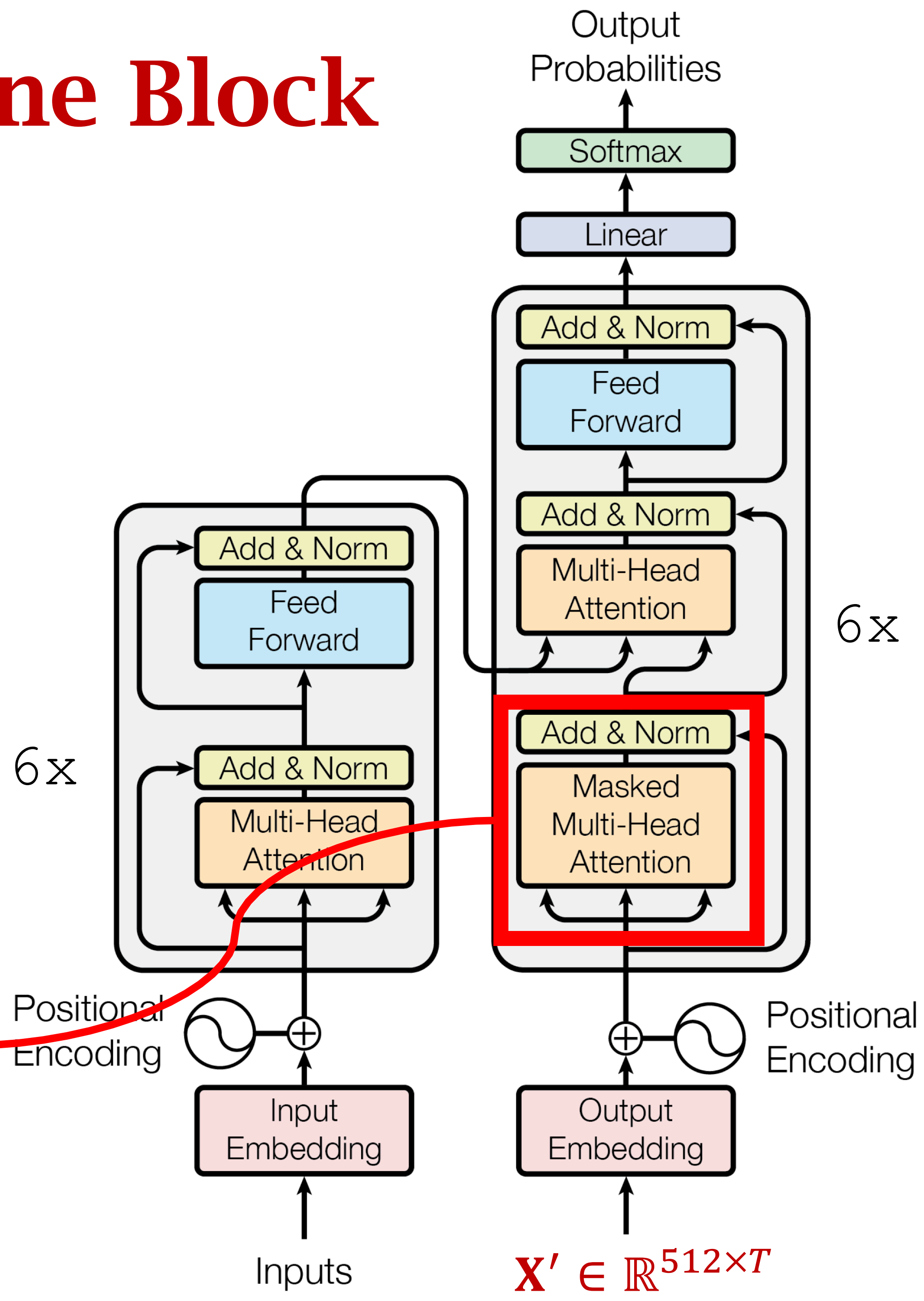




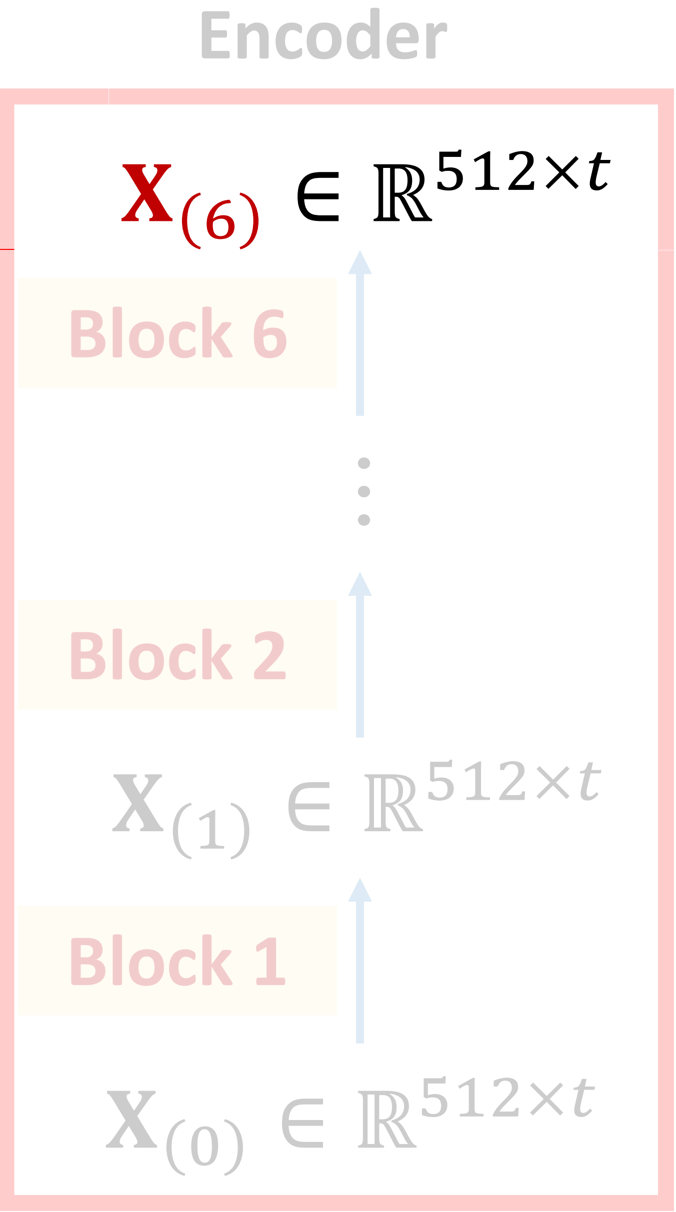
Decoder of Transformer

Decoder Network: One Block

- Similar to encoder.
- Set $\mathbf{Q} = \mathbf{K} = \mathbf{V} = \mathbf{X}'$.

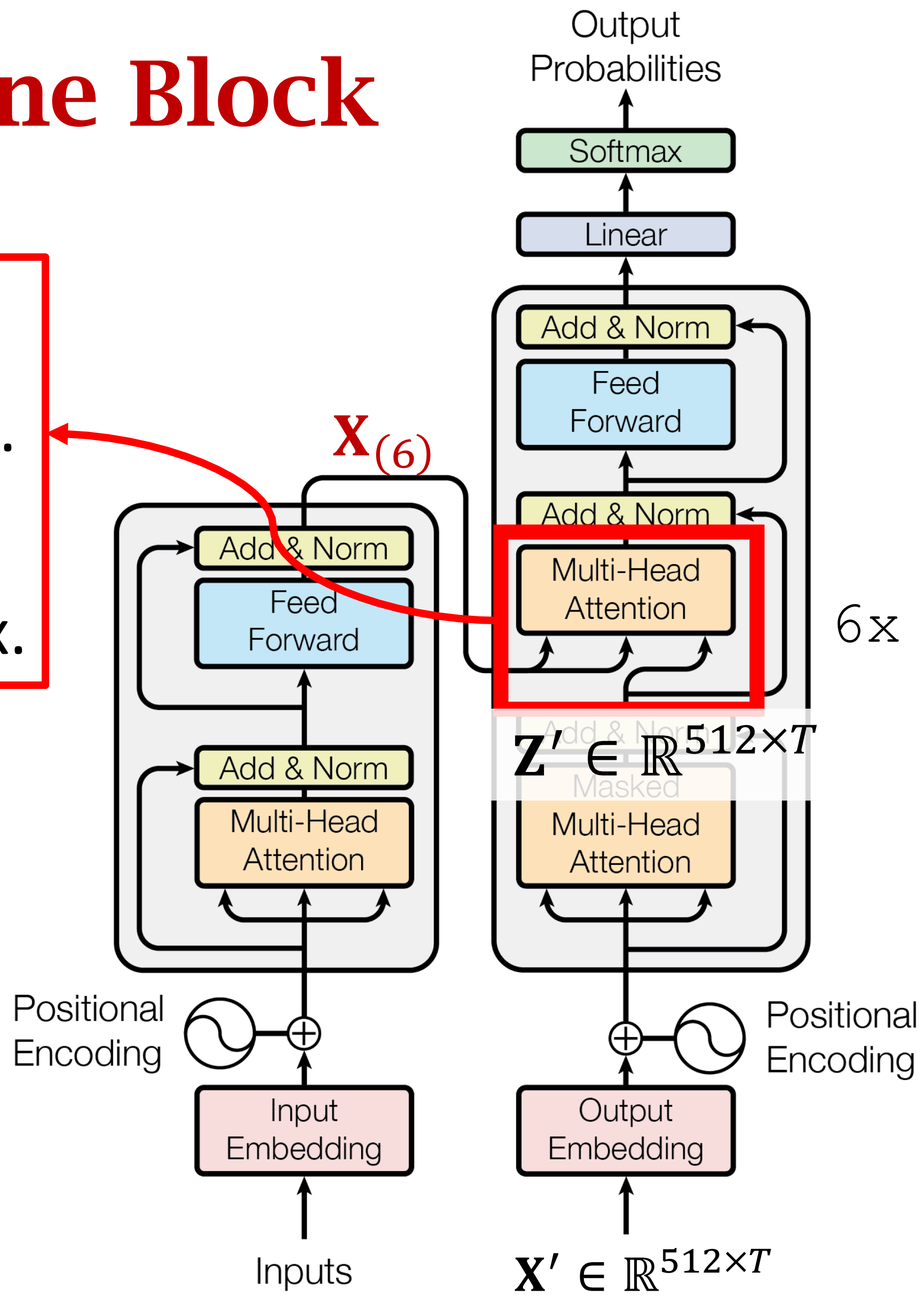


Decoder Network: One Block

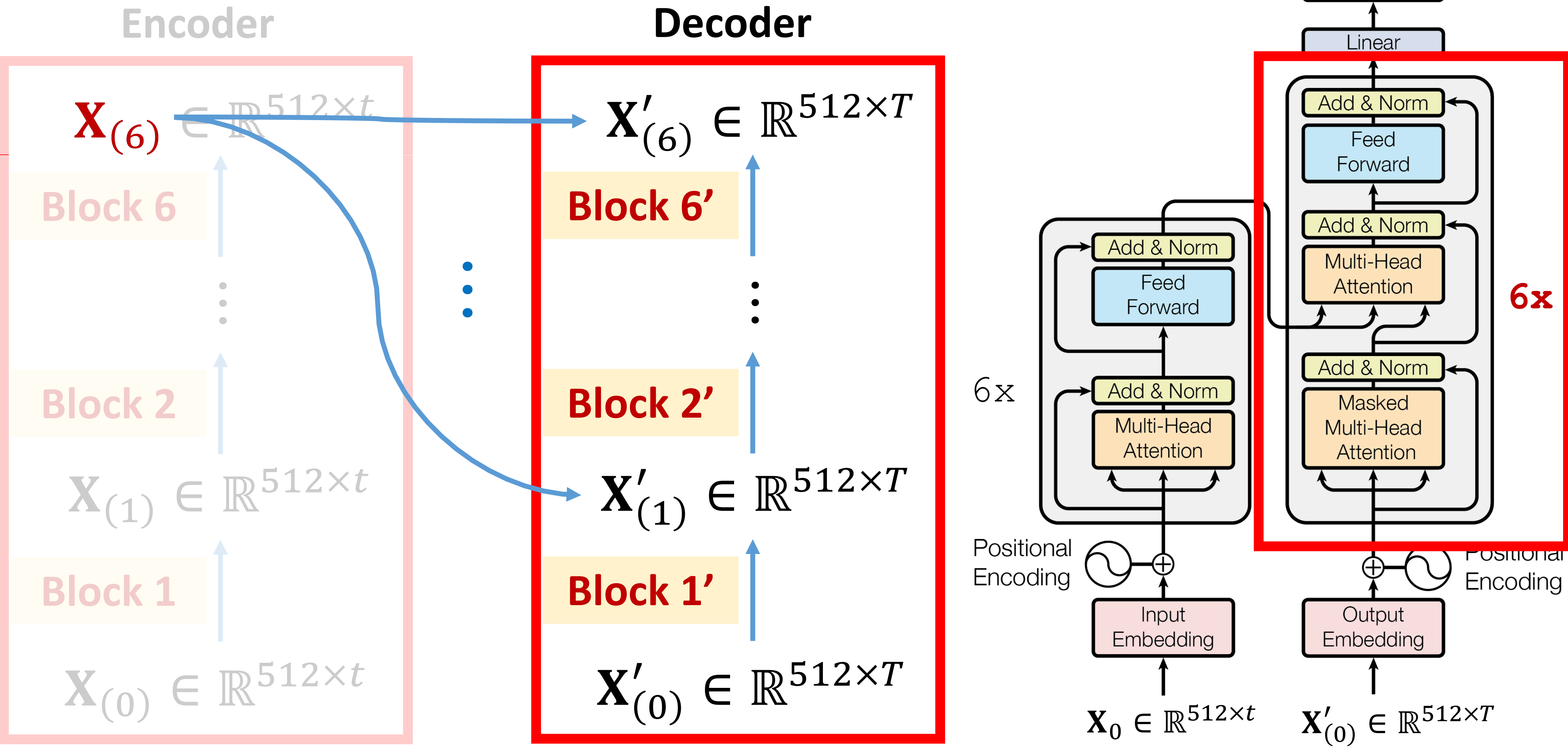


- Set $\mathbf{Q} = \mathbf{Z}' \in \mathbb{R}^{512\times T}$.
- $\mathbf{K} = \mathbf{V} = \mathbf{X}_{(6)} \in \mathbb{R}^{512\times t}$.
- Multi-head attention outputs a $512\times T$ matrix.

- Similar to encoder.
- Set $\mathbf{Q} = \mathbf{K} = \mathbf{V} = \mathbf{X}'$.

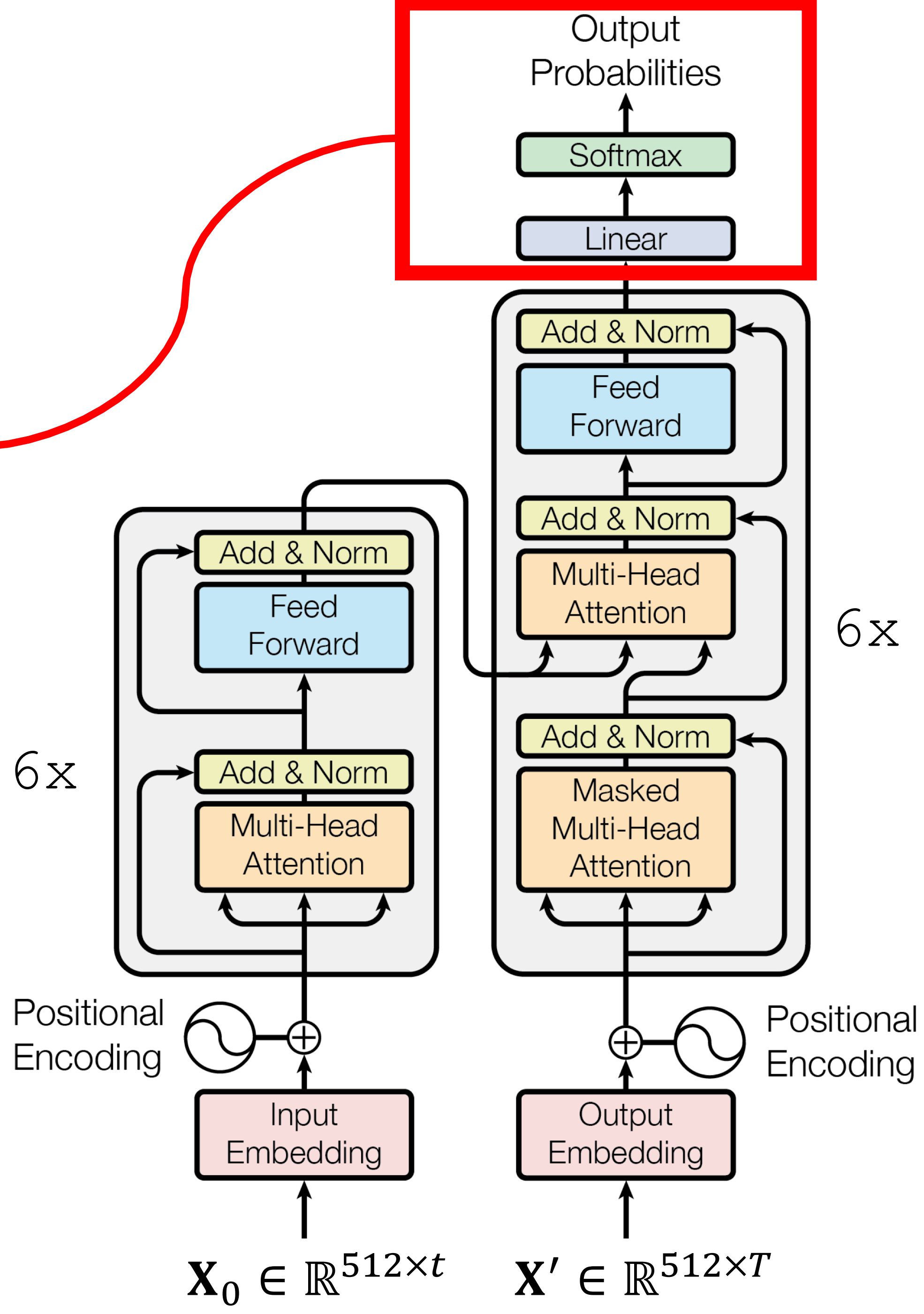


Decoder Network



Decoder Network

- Output a distribution over the vocabulary.
- Compare the distribution with the one-hot encode of the label.
- ➔ Loss.
- ➔ Gradient.
- ➔ Update model parameters.



Summary

Summary

- Transformer model is not RNN.
- Transformer is based on attention and self-attention.
- Upside: Outperform all the state-of-the-art RNN models.
- Downside: Much more expensive than RNN models.

- Read the original paper: Vaswani et al. Attention Is All You Need. In *NIPS*, 2017.
- Google "*transformer model explained*" and read the articles.

Key Concept: Multi-Head Attention

- Inputs: query $\mathbf{Q}$, key $\mathbf{K}$, and value $\mathbf{V}$.
- Linear maps: $\widetilde{\mathbf{Q}} = \mathbf{W}_q \mathbf{Q}$, $\widetilde{\mathbf{K}} = \mathbf{W}_k \mathbf{K}$, and $\widetilde{\mathbf{V}} = \mathbf{W}_v \mathbf{V}$.
- Single-head attention:

$$\mathbf{C} = \mathrm{attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \widetilde{\mathbf{V}} \cdot \mathrm{softmax}\left(\widetilde{\mathbf{K}}^T \widetilde{\mathbf{Q}}\right).$$

Key Concept: Multi-Head Attention

- Inputs: query $\mathbf{Q}$, key $\mathbf{K}$, and value $\mathbf{V}$.
- Linear maps: $\tilde{\mathbf{Q}} = \mathbf{W}_q \mathbf{Q}$, $\tilde{\mathbf{K}} = \mathbf{W}_k \mathbf{K}$, and $\tilde{\mathbf{V}} = \mathbf{W}_v \mathbf{V}$.
- Single-head attention:

$$\mathbf{C} = \text{attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \tilde{\mathbf{V}} \cdot \text{softmax}\left(\tilde{\mathbf{K}}^T \tilde{\mathbf{Q}}\right).$$

- Multi-head attention:
  - Repeat $\text{attn}(\mathbf{Q}, \mathbf{K}, \mathbf{V})$ using different parameters $\mathbf{W}_q, \mathbf{W}_v, \mathbf{W}_v$.
  - Get $\mathbf{C}^{[1]}, \mathbf{C}^{[2]}, \cdots, \mathbf{C}^{[m]} \in \mathbb{R}^{d_z \times t}$.
  - Concatenate the m matrices to get $\tilde{\mathbf{C}} \in \mathbb{R}^{m d_z \times t}$.

Attention in the encoder:

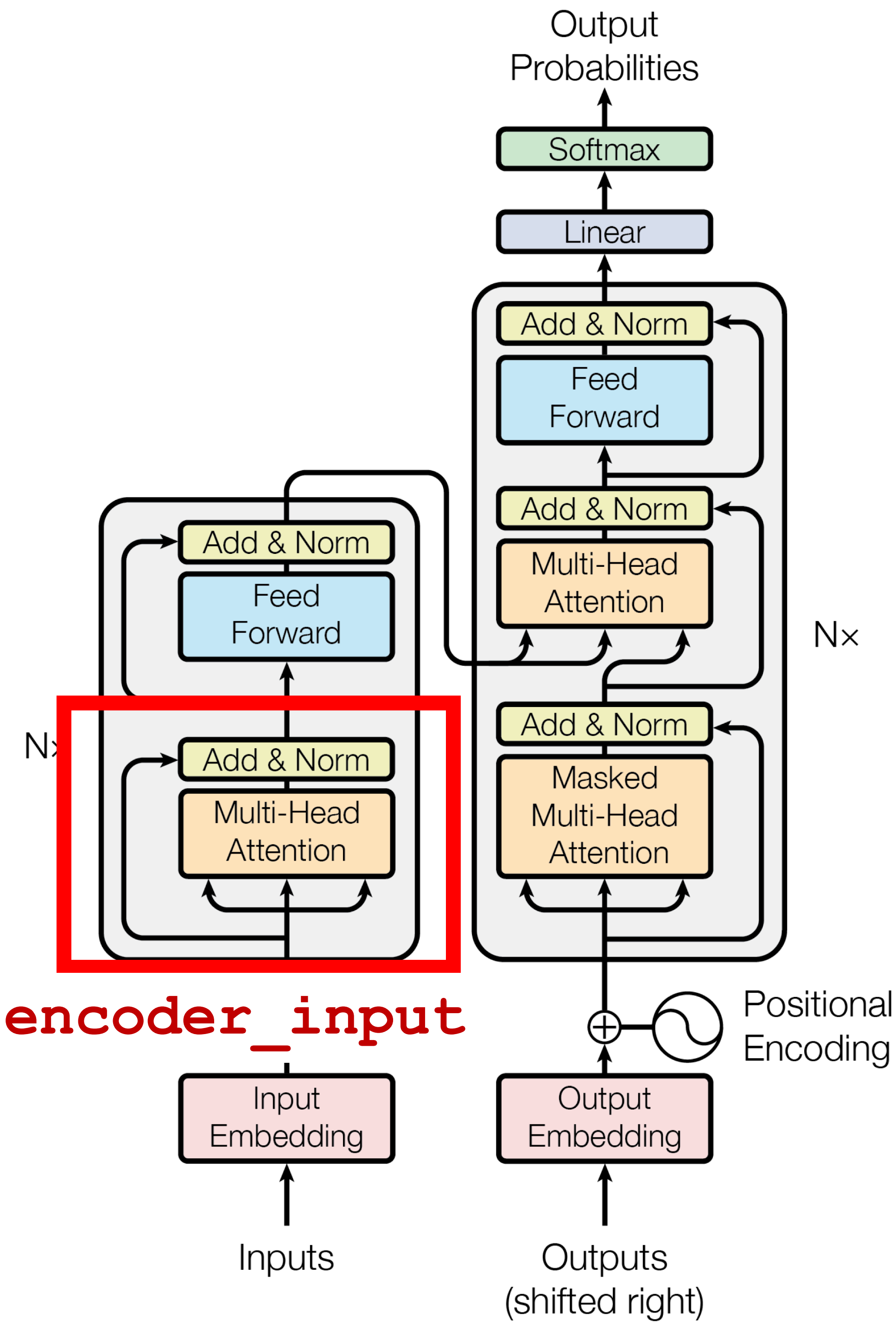
- $\mathbf{Q} = \mathbf{K} = \mathbf{V} =$ `encoder_input`.

1^{st} attention in the decoder:

- $\mathbf{Q} = \mathbf{K} = \mathbf{V} =$ `decoder_input`.

2^{nd} attention in the decoder

- $\mathbf{Q} =$ `decoder_input`
- $\mathbf{K} = \mathbf{V} =$ `encoder_output`.



Attention in the encoder:

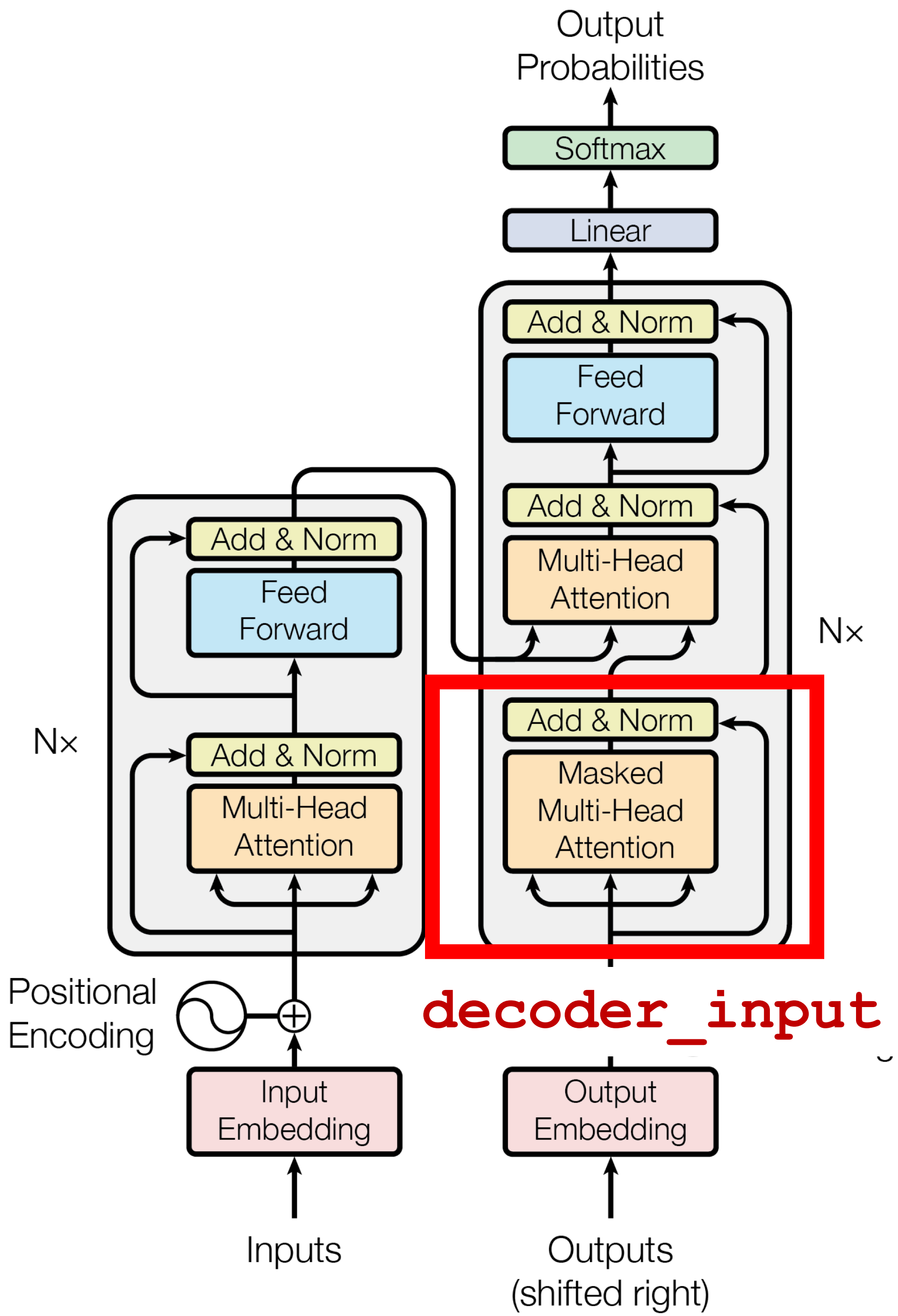
- $Q = K = V =$ encoder_input.

1^{st} attention in the decoder:

- $Q = K = V =$ decoder_input.

2^{nd} attention in the decoder

- $Q =$ decoder_input
- $K = V =$ encoder_output.



Attention in the encoder:

- Q = K = V = encoder_input.

1st attention in the decoder:

- Q = K = V = decoder_input.

2nd attention in the decoder

- Q = decoder_input
- K = V = encoder_output.