Attention Mechanism and Transformer Architecture

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Review of RNN

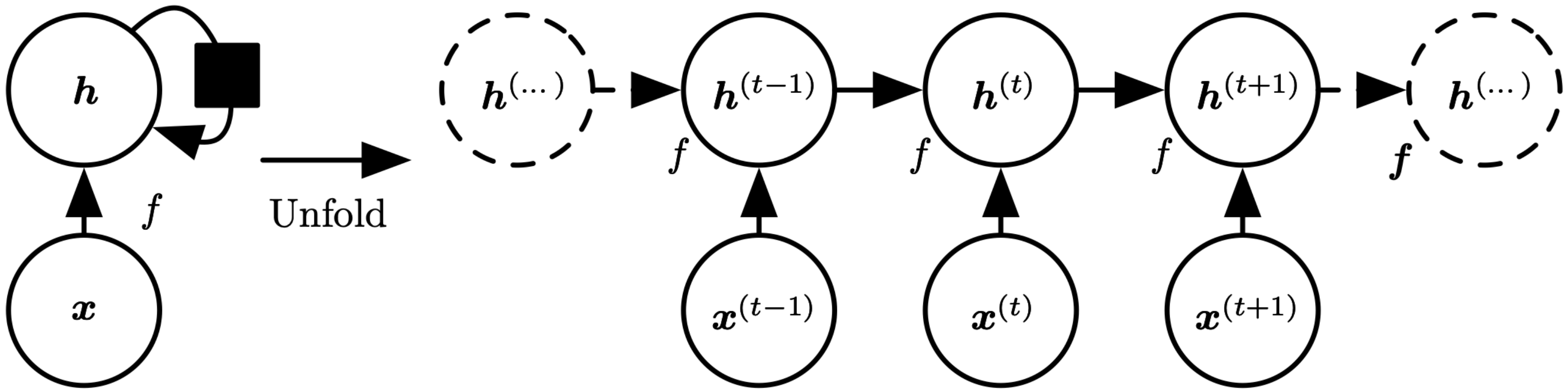


Figure 10.2

Figure from (Goodfellow 2016)

How to use RNN for sequence-to-sequence task?

- **Example**: Translation between French and English
- **Option 1:** one-to-one input/output RNN
  - Problem: Sequences could have different lengths.
  - Problem: The order of words is not the same in French and English.

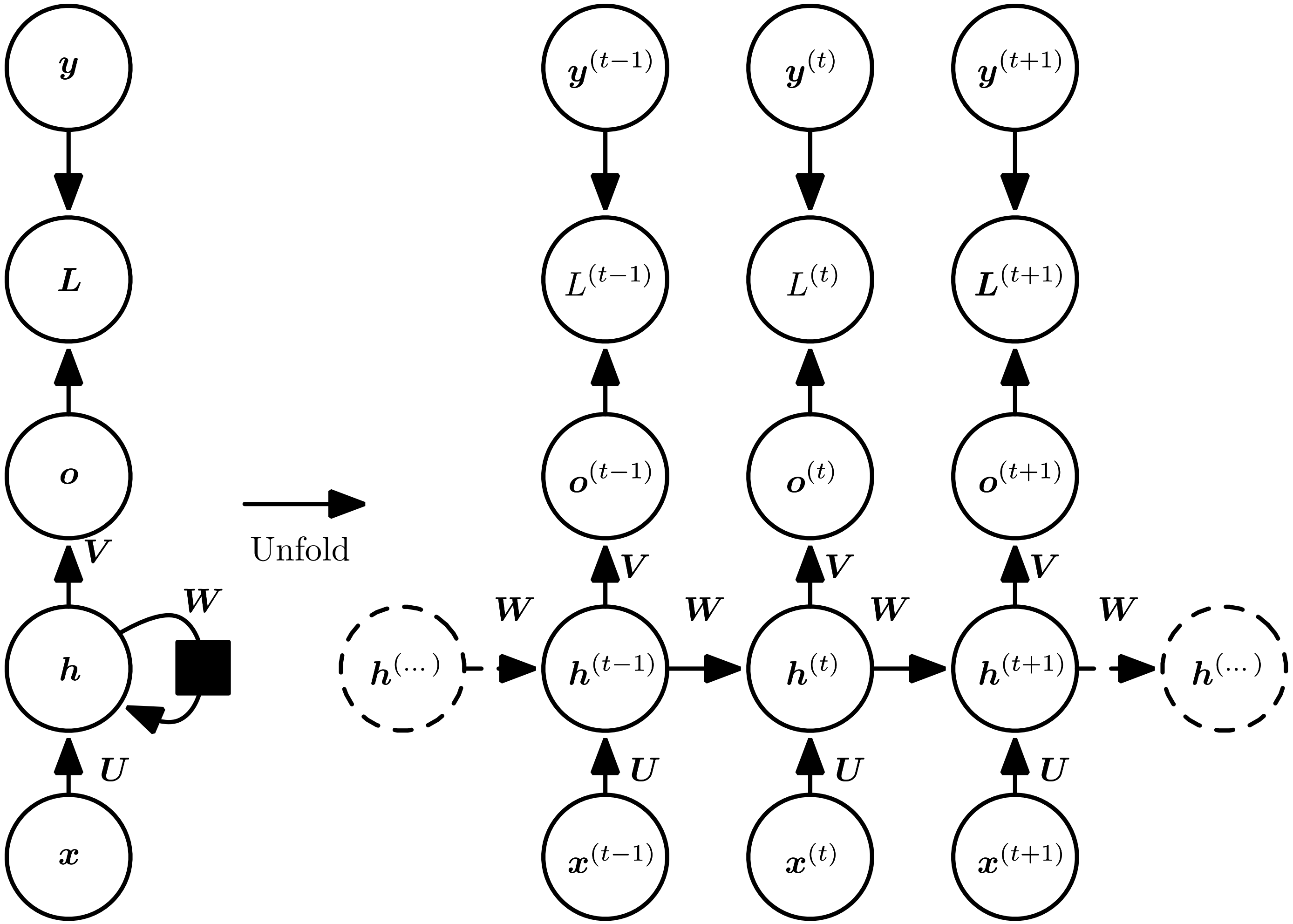


Figure from (Goodfellow 2016)

How to use RNN for sequence-to-sequence task?

- **Example**: Translation between French and English
- **Option 2:** encoder-decoder structure
  - Hidden state **s** in the decoder

$$s_t = g(s_{t-1}, y_{t-1}, c)$$

  - Problem: difficult to encode a whole input sentence into a single fixed-length context vector **c**, especially for long sentences

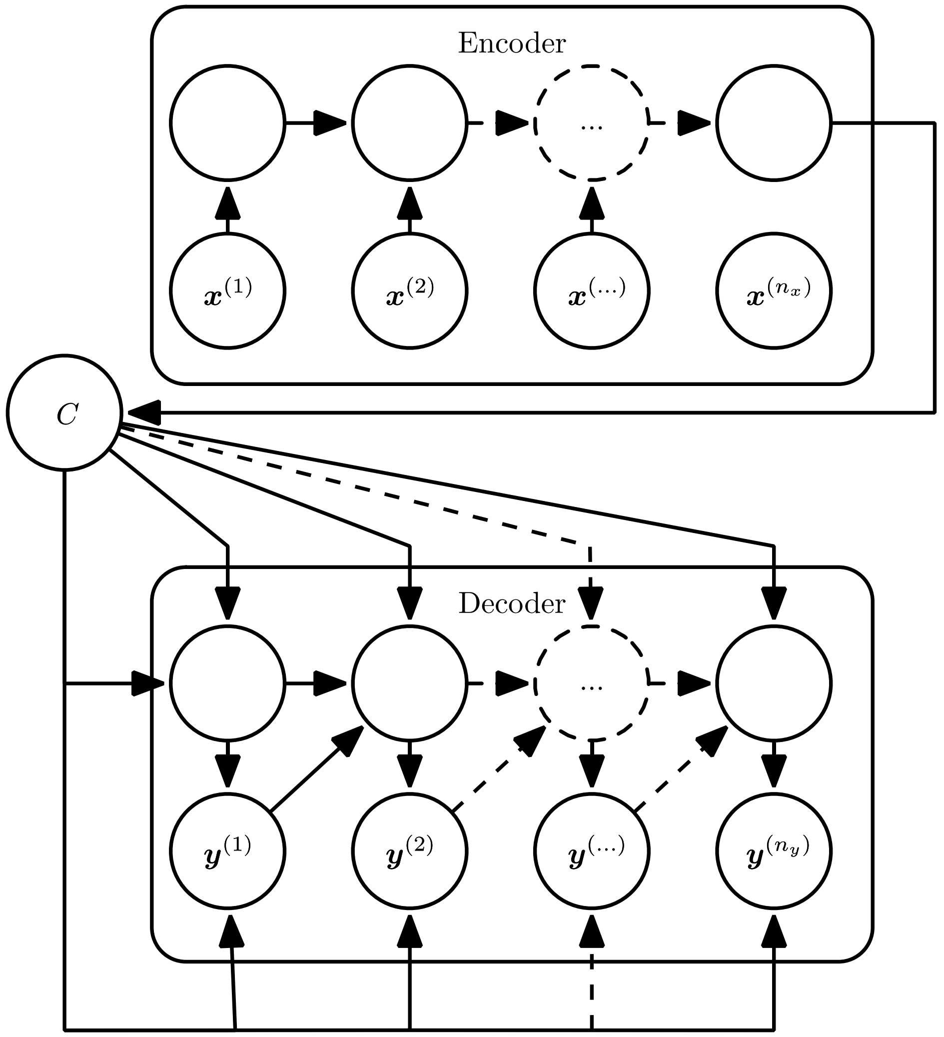


Figure from (Goodfellow 2016)

Attention mechanism in sequence-to-sequence task

- **Example**: Translation between French and English
- Attention mechanism to learn distinct context vectors:
    - Hidden state **s** in the decoder

$$s_t = g(s_{t-1}, y_{t-1}, \boxed{c_t})$$

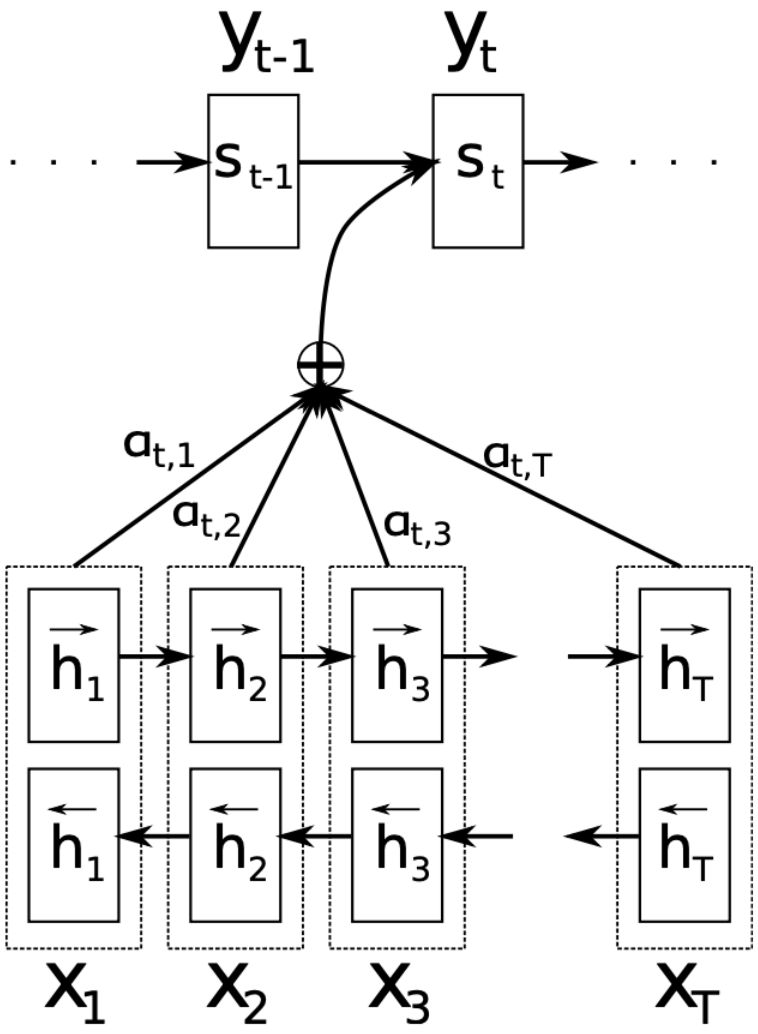


Figure from (Bahdanau et al. 2015)

Attention mechanism in sequence-to-sequence task

- **Example**: Translation between French and English
- Attention mechanism to learn distinct context vectors:
  - Hidden state **s** in the decoder

$$s_t = g(s_{t-1}, y_{t-1}, \boxed{c_t})$$

where $$c_i = \sum_{j=1}^{T_x} \alpha_{ij} h_j \quad \alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})},$$

$$e_{ij} = a(s_{i-1}, h_j)$$

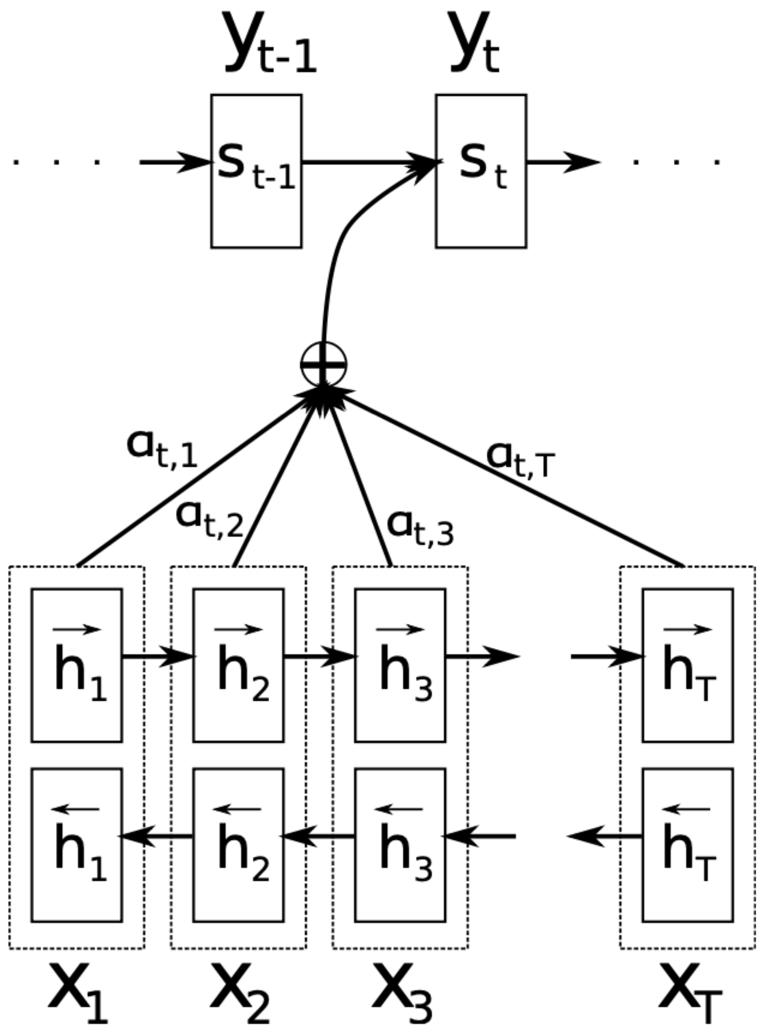


Figure from (Bahdanau et al. 2015)

Attention mechanism in sequence-to-sequence task

- Alignment model scores how well the inputs around position j and the output at position i match:

$$e_{ij} = a(s_{i-1}, h_j)$$

- The attention weights are normalized via softmax such that $\sum_j \alpha_{ij} = 1$

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})},$$

- In other words, the attention mechanism determines which encoder outputs the network should "focus" on

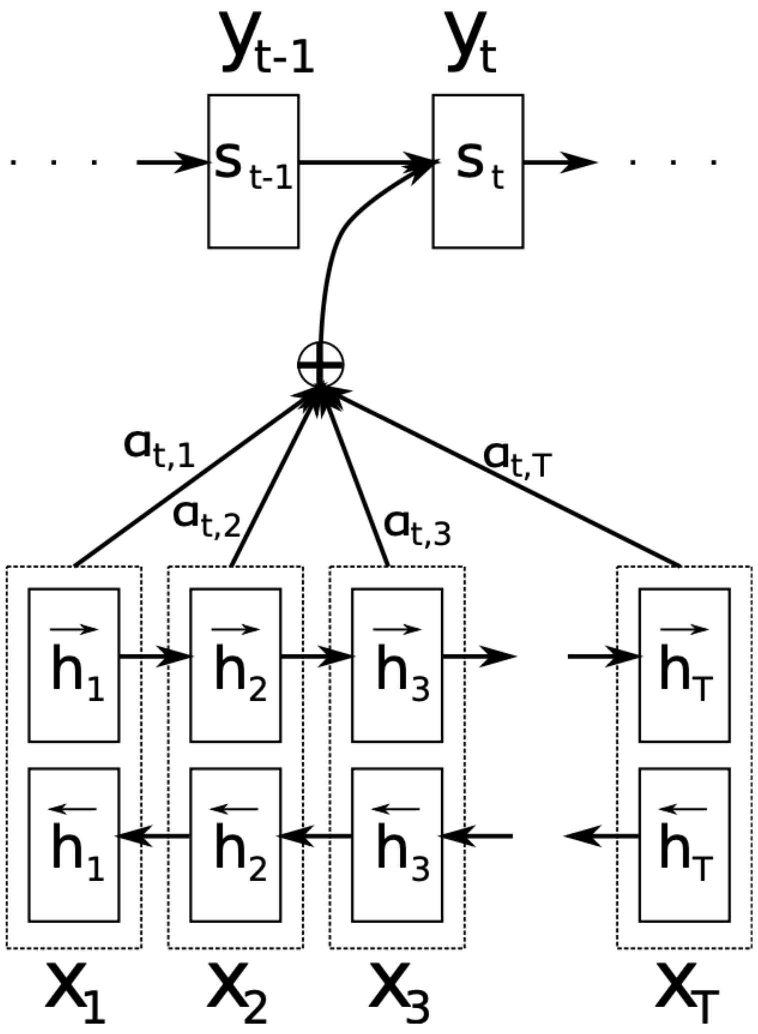
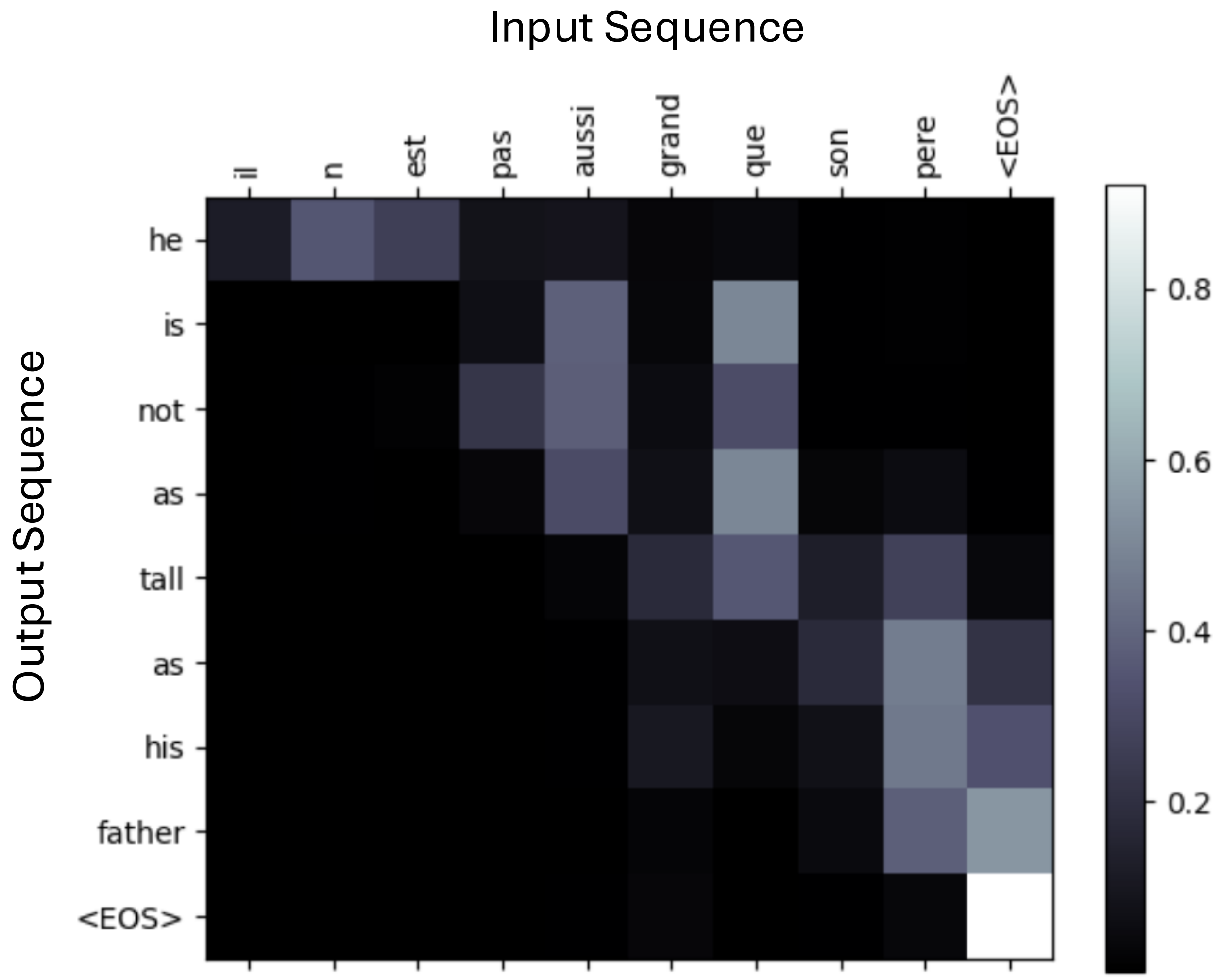


Figure from (Bahdanau et al. 2015)

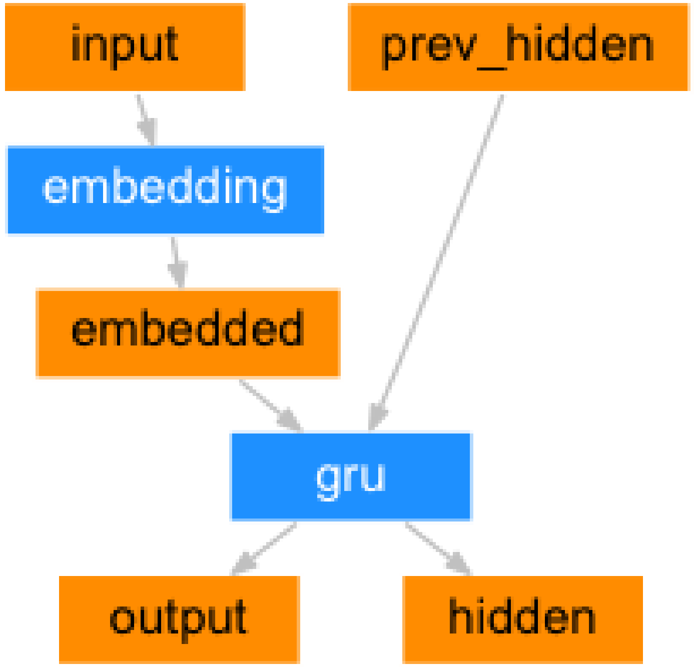
Visualization of attention weights as interpretation

- Visualization of the attention weights α shows what the model pays attention to when making the prediction.



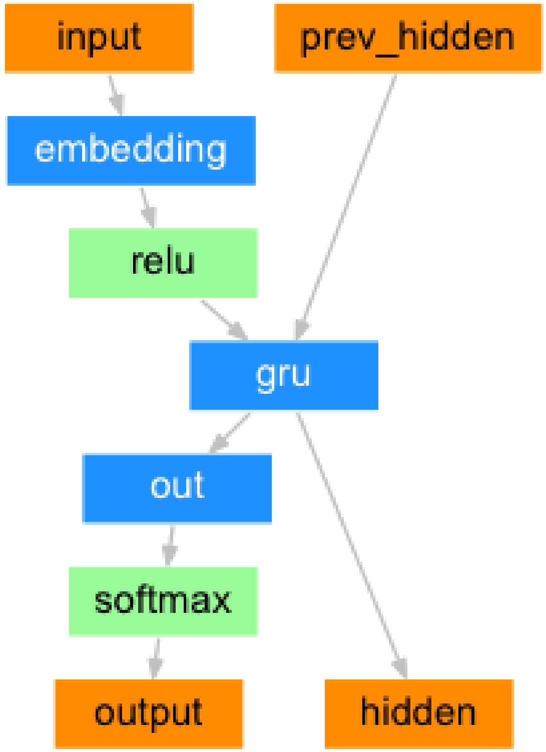
Demo of sequence to sequence task

- **Example**: Translation between French and English
  - Tutorial from https://pytorch.org/tutorials/intermediate/seq2seq_translation_tutorial.html
  - **Encoder** is simple RNN



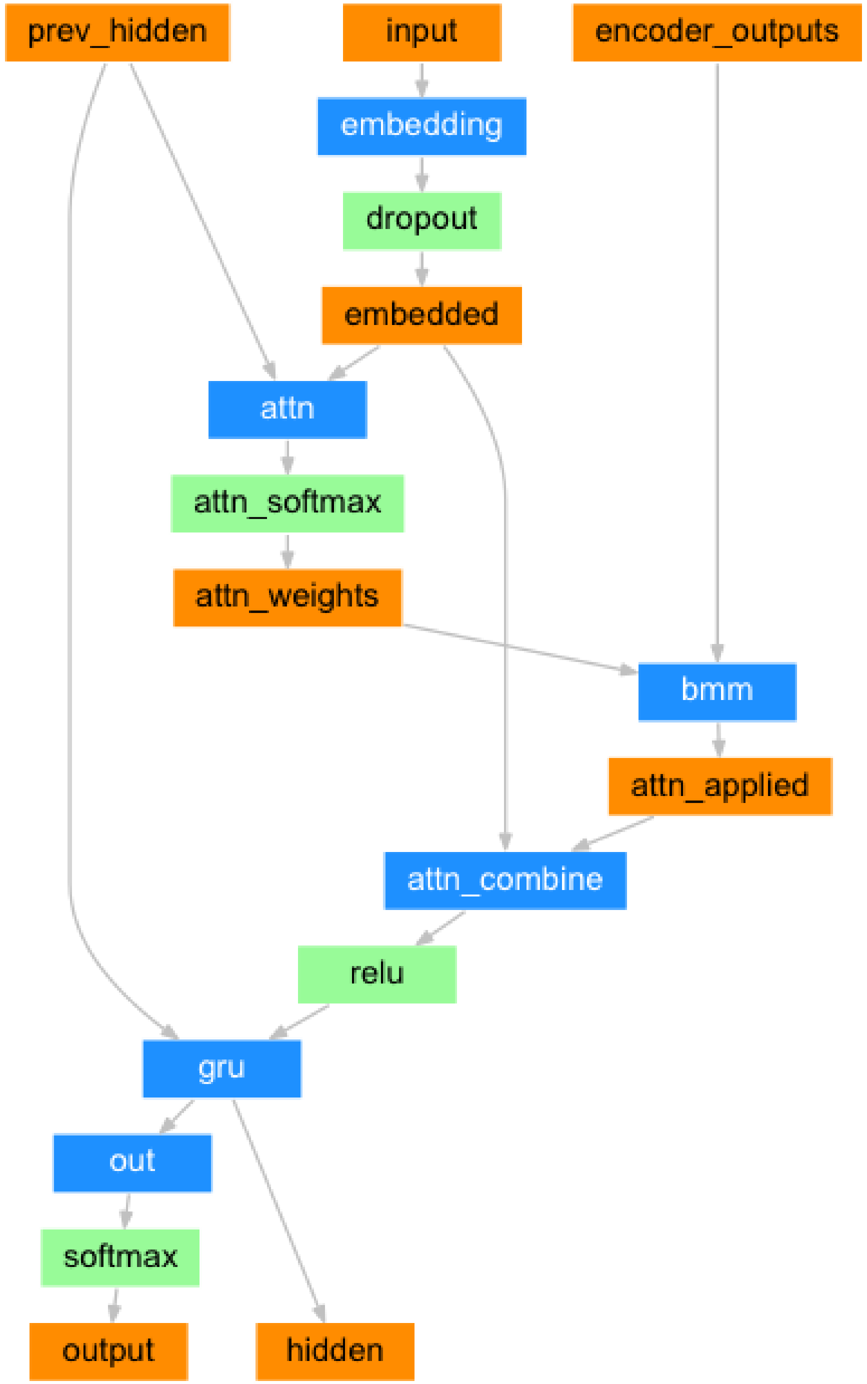
Demo of sequence to sequence task

- **Example**: Translation between French and English
  - Tutorial from https://pytorch.org/tutorials/intermediate/seq2seq_translation_tutorial.html
  - **RNNdecoder** includes a simple RNN



Demo of sequence to sequence task

- **Example**: Translation between French and English
  - Tutorial from https://pytorch.org/tutorials/intermediate/seq2seq_translation_tutorial.html
  - **AttnDecoderRNN** includes the attention mechanism



Our seq-2-seq attention is a special case of this more general attention mechanism

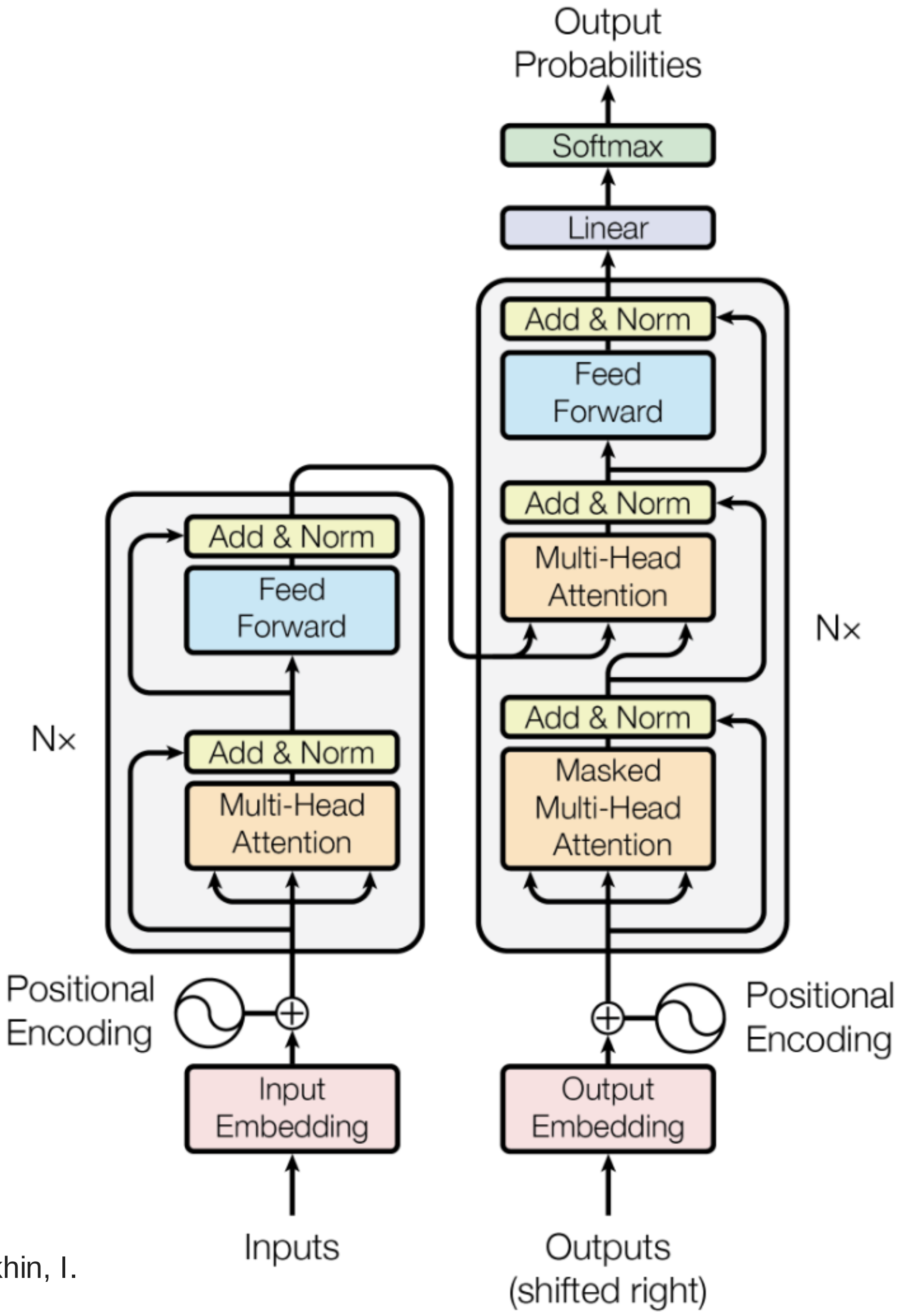
- The output of attention is a weighted average of the values

$$A(q, K, V) = \sum_i \alpha_i v_i = \sum_i \left(\frac{\exp\big(e(q, k_i)\big)}{\sum_j \exp\Big(e\big(q, k_j\big)\Big)} \right) v_i$$

  - q is the **query** input, K is the key matrix, V is the value matrix
  - α_i is the **attention weight** for the i-th value
  - $e(q, k_i)$ is the **attention score** (pre-softmax) based on the i-th key

Transformer

- No RNN structure, only attention, parallel computing
- Long-range interaction
- Positional encoding
- Multi-head attention



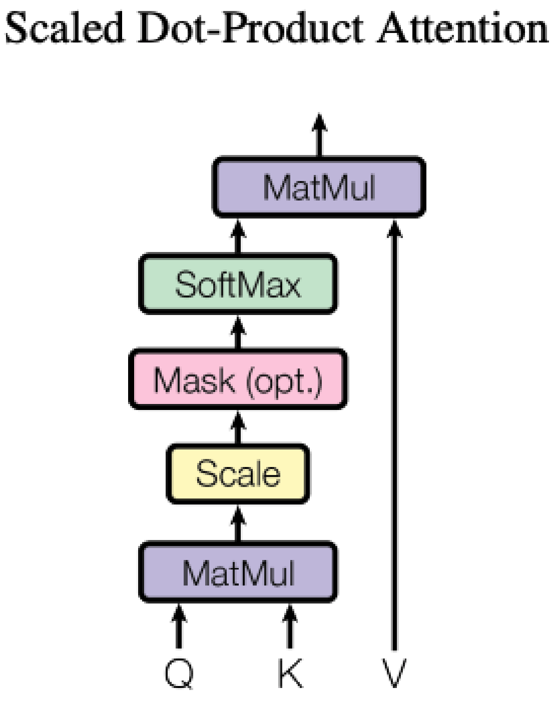
Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. *Advances in neural information processing systems*, *30*.

Scaled Dot-Product Attention

- $X = [x_1, x_2, \dots, x_L]^T \in \mathbb{R}^{n \times d_{model}}$, n is sequence length
- Self attention to compute Q, K and V
  - $Q = XW_Q \in \mathbb{R}^{n \times d_k}$
  - $K = XW_K \in \mathbb{R}^{n \times d_k}$
  - $V = XW_V \in \mathbb{R}^{n \times d_v}$
- Dot-product attention with a scaling factor $\frac{1}{\sqrt{d_k}}$

$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

- Additive attention vs. dot-product attention



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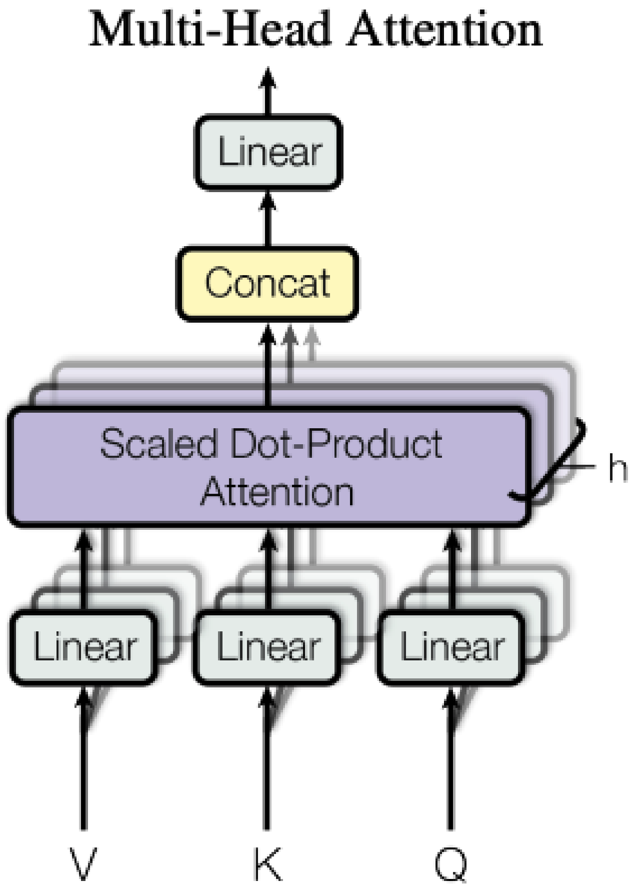
Multi-head attention

- Use h attention modules and concatenate their outputs

$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head_1}, ..., \mathrm{head_h})W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

- Allowing the model to jointly attend to information from different representation subspaces at different positions

- Reduced dimension of each head



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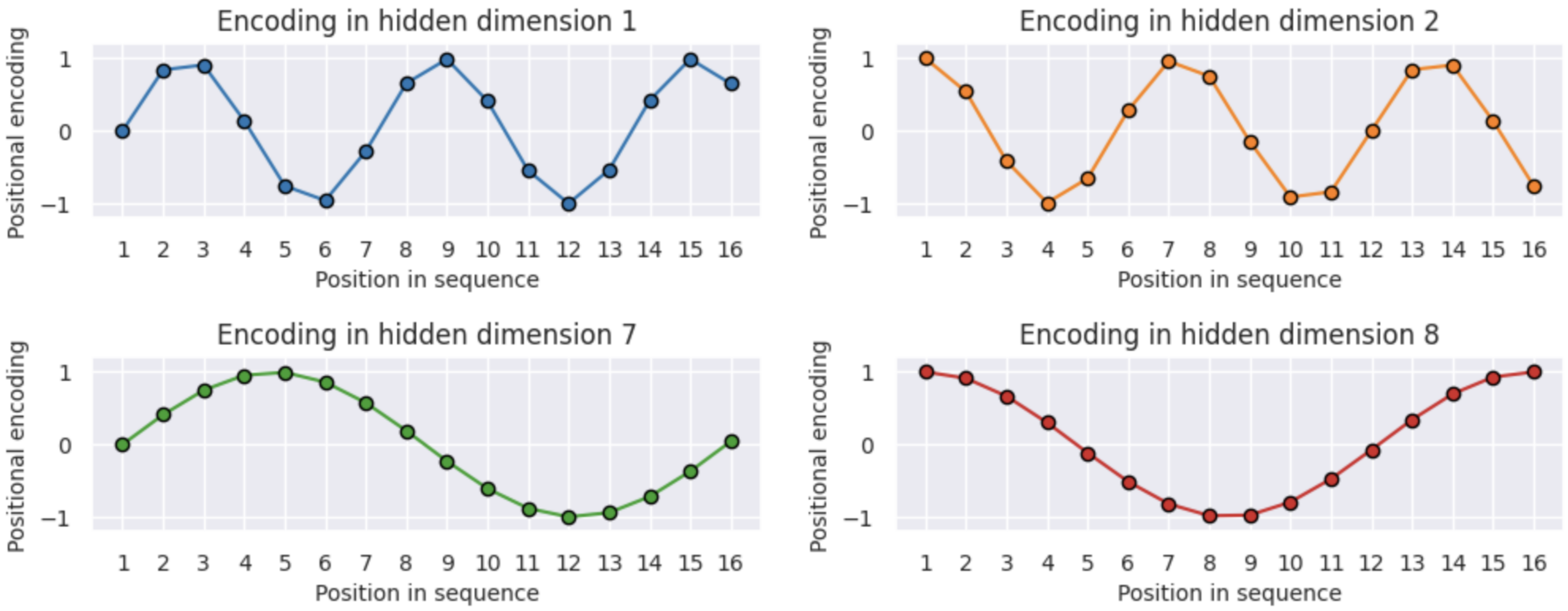
Positional Encoding

- Positional encoding has the same dimension d_{model} as the word embedding x
- Alternating between sine and cosine functions of different frequencies:

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$

$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

where pos is the position and i is the dimension



Positional Encoding

- The wavelengths form a geometric progression from 2π to $10000 \cdot 2\pi$.

- This enables relative and absolute positioning information to be encoded
  - Enables relative positioning because for any k, PE_{pos+k} can be represented as a linear function of PE_{pos}

- There are other choices of positional encodings, either learned and fixed. Refer to Gehring, Jonas, et al. "Convolutional sequence to sequence learning." International conference on machine learning. PMLR, 2017.

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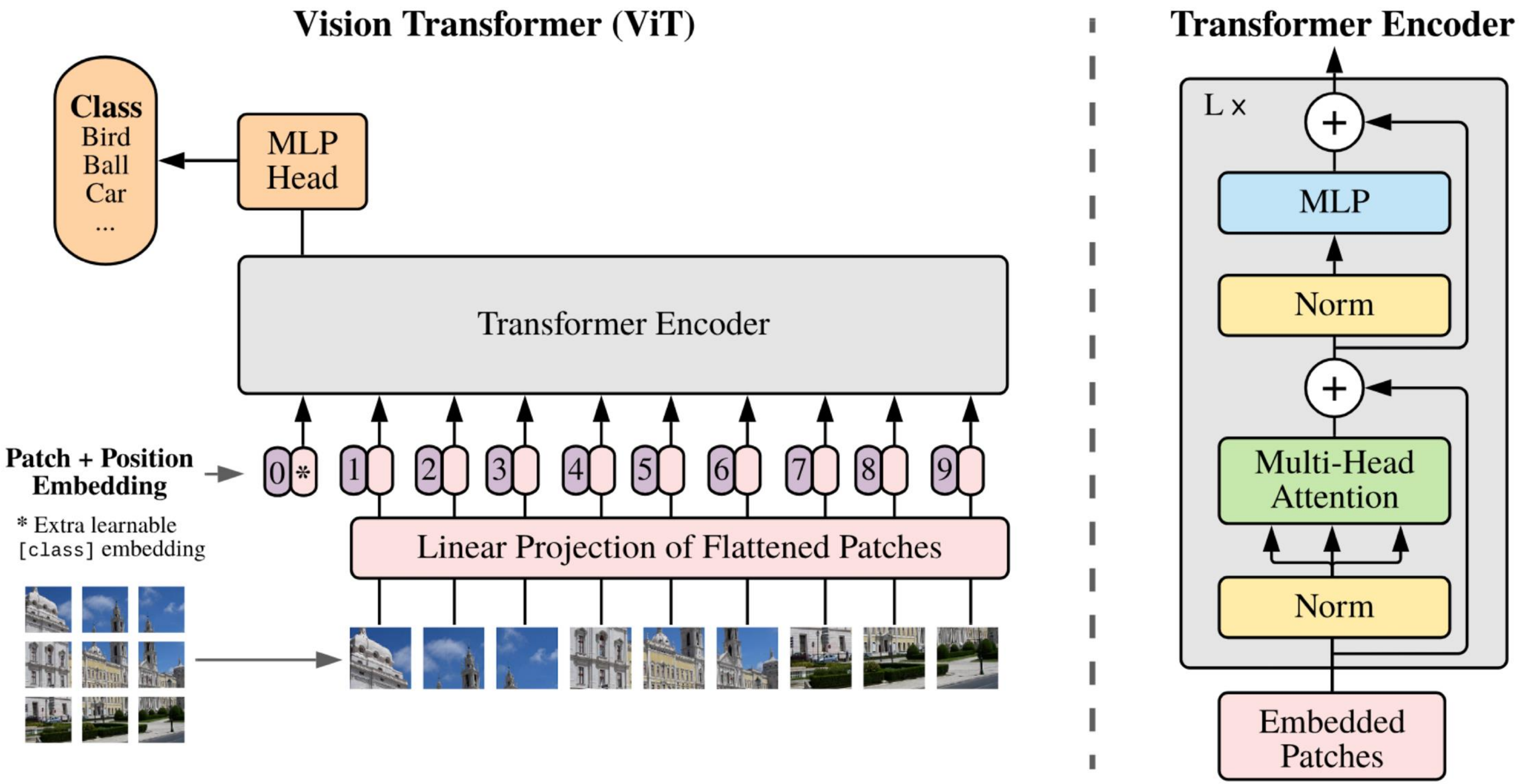
Transformers are applicable to various contexts



Dosovitskiy, Alexey, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani et al. "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale." In International Conference on Learning Representations. 2020.