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Escuela de Ciencias Aplicadas e Ingeniería

ST7003 Procesamiento Natural del Lenguaje

Lecture03c – Attention is all you need

Contenido

1. Token embeddings
2. Positional encodings
3. Sequence modeling
4. Recurrent neural networks
5. Attention

Creating token embeddings

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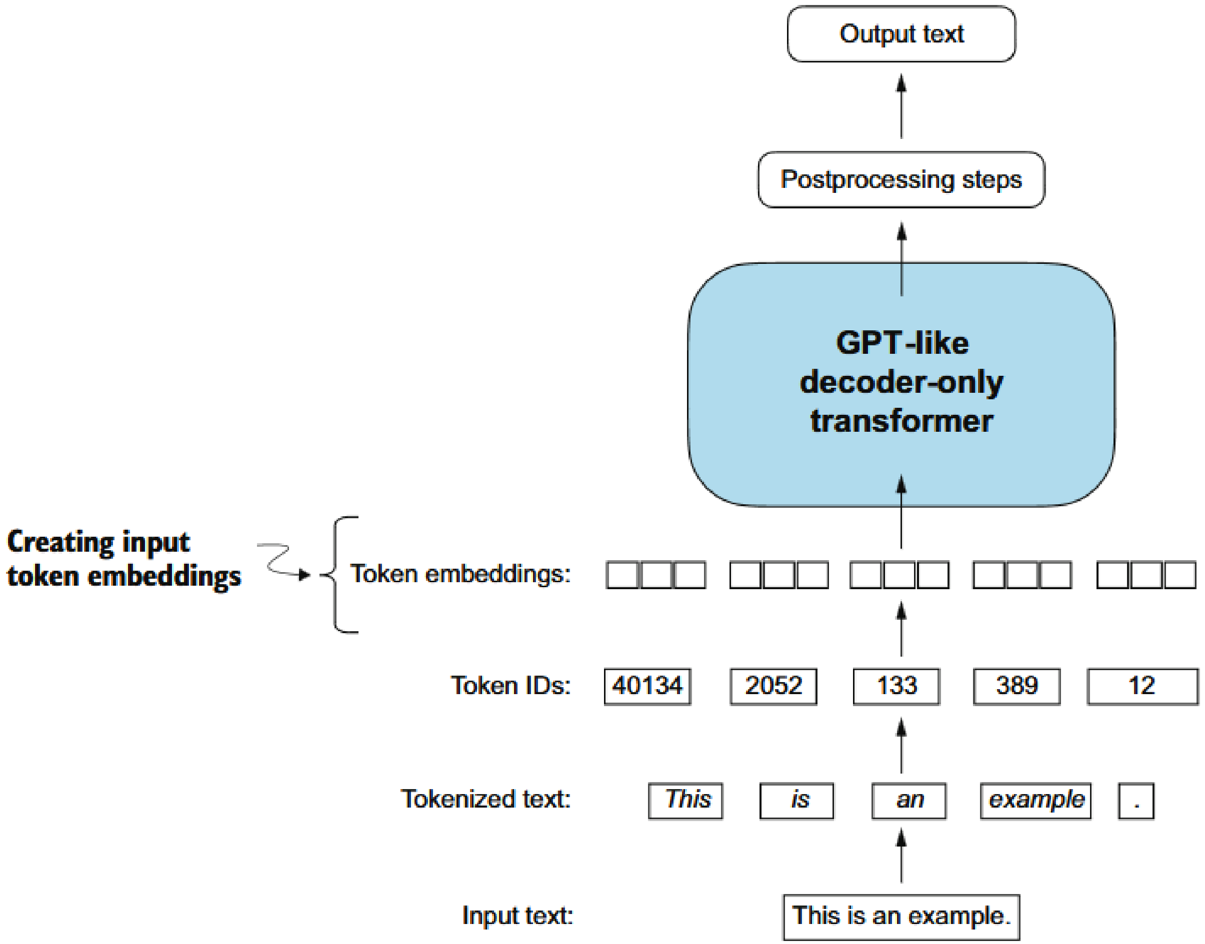

Creating token embeddings

Embedding layers: An efficient way of performing matrix multiplication when working with one-hot encoded vectors.

```
import torch

torch.manual_seed(123);
```

```
idx = torch.tensor([2, 3, 1]) # 3 training examples

num_idx = max(idx)+1
out_dim = 5
```

Suppose we want embeddings of size 5

Input dimension of a one-hot encoded vector is the number of indices (the highest index + 1)

Creating token embeddings

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```
import torch

torch.manual_seed(123);
```

```
idx = torch.tensor([2, 3, 1]) # 3 training examples

num_idx = max(idx)+1
out_dim = 5

embedding = torch.nn.Embedding(num_idx, out_dim)
embedding(idx)
```

```
tensor([[ 0.6957, -1.8061, -1.1589,  0.3255, -0.6315],
        [-2.8400, -0.7849, -1.4096, -0.4076,  0.7953],
        [ 1.3010,  1.2753, -0.2010, -0.1606, -0.4015]],
       grad_fn=<EmbeddingBackward0>)
```

Each training example has 5 feature values

Creating token embeddings

One-hot encoded ("sparse") representation of "S U N N Y"

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
S	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
N	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
N	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Y	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0

↓

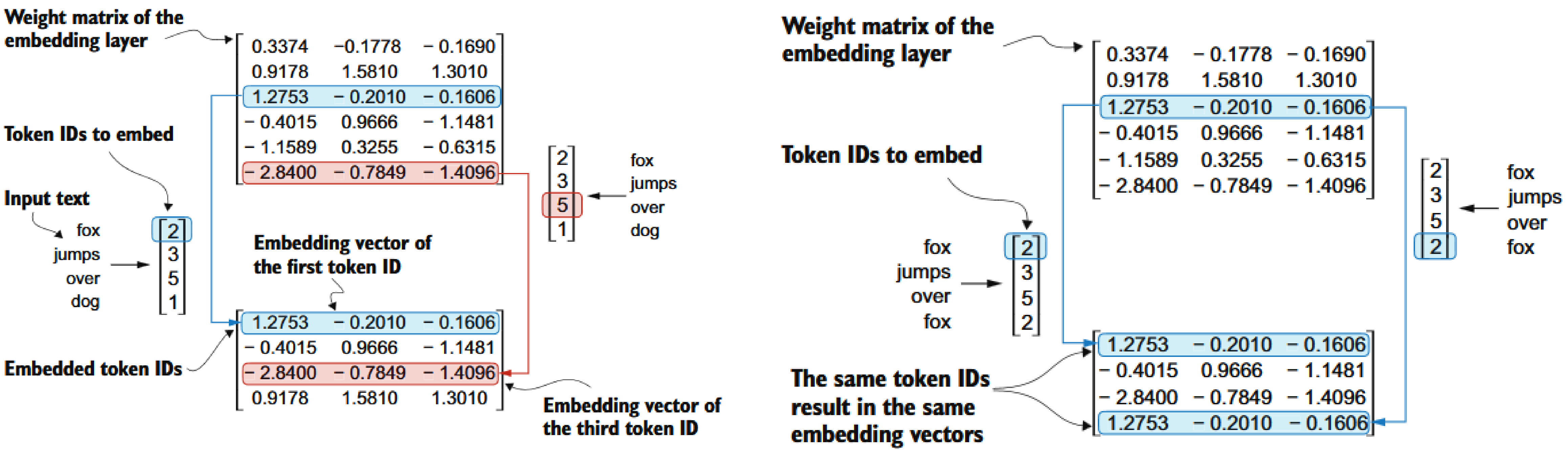
Embedded ("dense") representation of "S U N N Y"

```
[[0.9816, 0.7363, 0.5899],
 [0.2605, 0.3766, 0.3502],
 [0.7382, 0.9807, 0.4762],
 [0.6231, 0.8825, 0.8836]]
```

Embedding layer

```
  [[0.6912, 0.8765, 0.4939],
   [0.6342, 0.7481, 0.7717],
   [0.8395, 0.2128, 0.3696],
   [0.4900, 0.1509, 0.0689],
   [0.2587, 0.9171, 0.8670],
   [0.7213, 0.9922, 0.5701],
   [0.7598, 0.5231, 0.3666],
   [0.5150, 0.5216, 0.9682],
   [0.2248, 0.0261, 0.4427],
   [0.1818, 0.6863, 0.8713],
   [0.4192, 0.1566, 0.9004],
   [0.8102, 0.5741, 0.4241],
   [0.1116, 0.0466, 0.2786],
S  [0.9816, 0.7363, 0.5899],
   [0.9224, 0.3672, 0.6972],
   [0.1207, 0.3372, 0.2128],
   [0.0660, 0.1524, 0.8440],
   [0.2162, 0.5640, 0.0988],
U  [0.2605, 0.3766, 0.3502],
   [0.2334, 0.4757, 0.7581],
N  [0.7382, 0.9807, 0.4762],
   [0.2369, 0.8102, 0.8798],
   [0.6932, 0.2671, 0.8018],
   [0.9593, 0.5302, 0.4290],
Y  [0.6231, 0.8825, 0.8836],
   [0.4623, 0.8503, 0.7279]]
```

Creating token embeddings



Sentence embeddings

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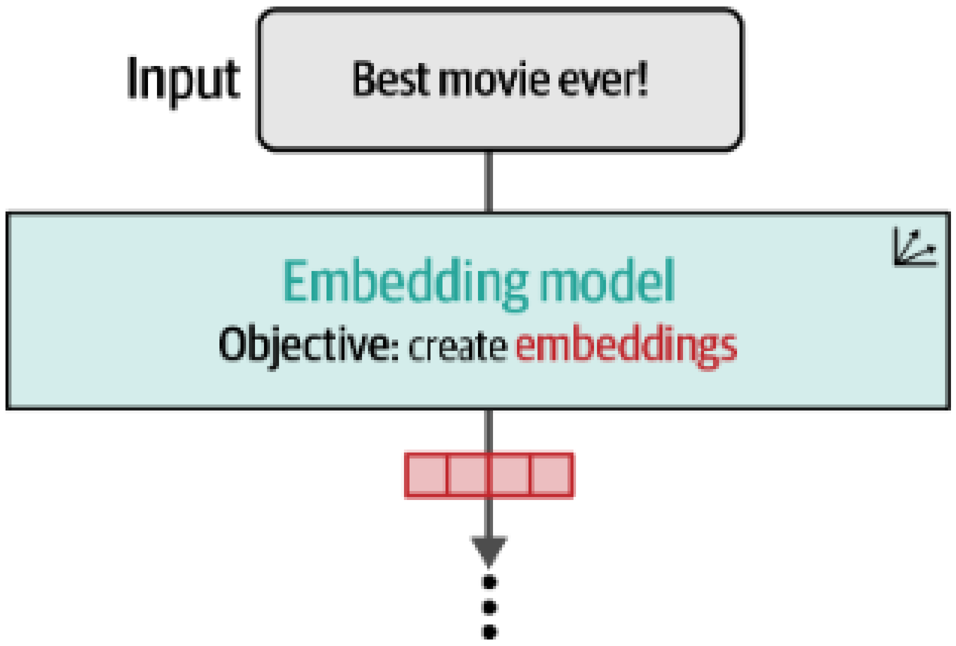
Task: Aggregate token embeddings in a sentence to form a **unique sentence representation.**



Encoding word positions

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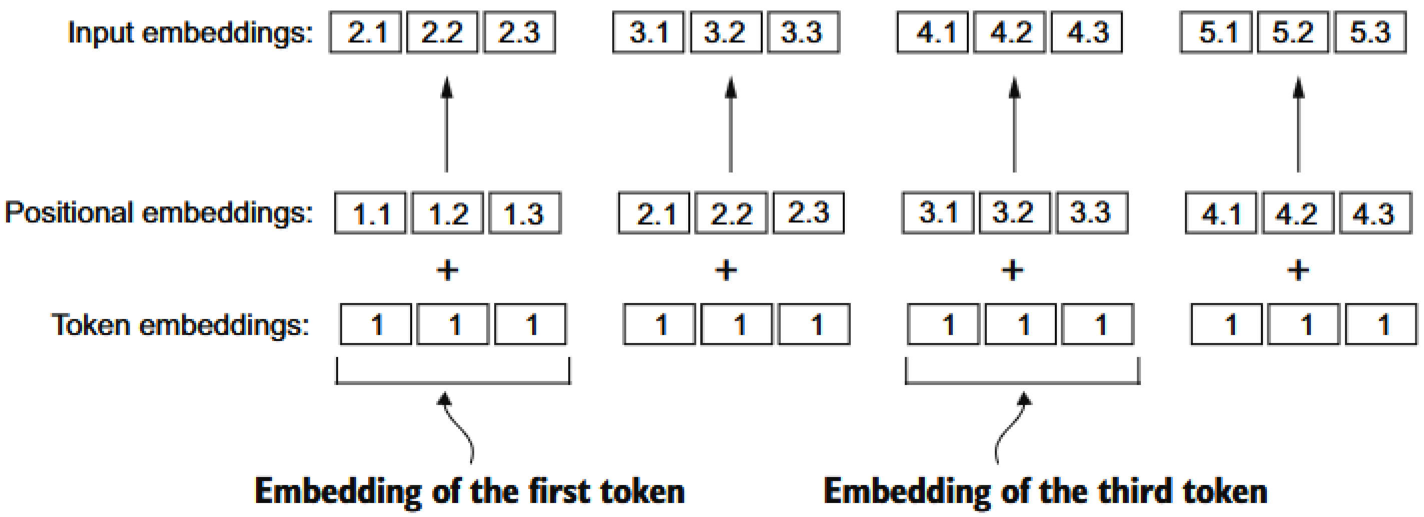

OpenAI: Positional embeddings are learnable parameters.
Llama, DeepSeek: Rotational Positional Embeddings – RoPE

Sinusoidal positional embeddings

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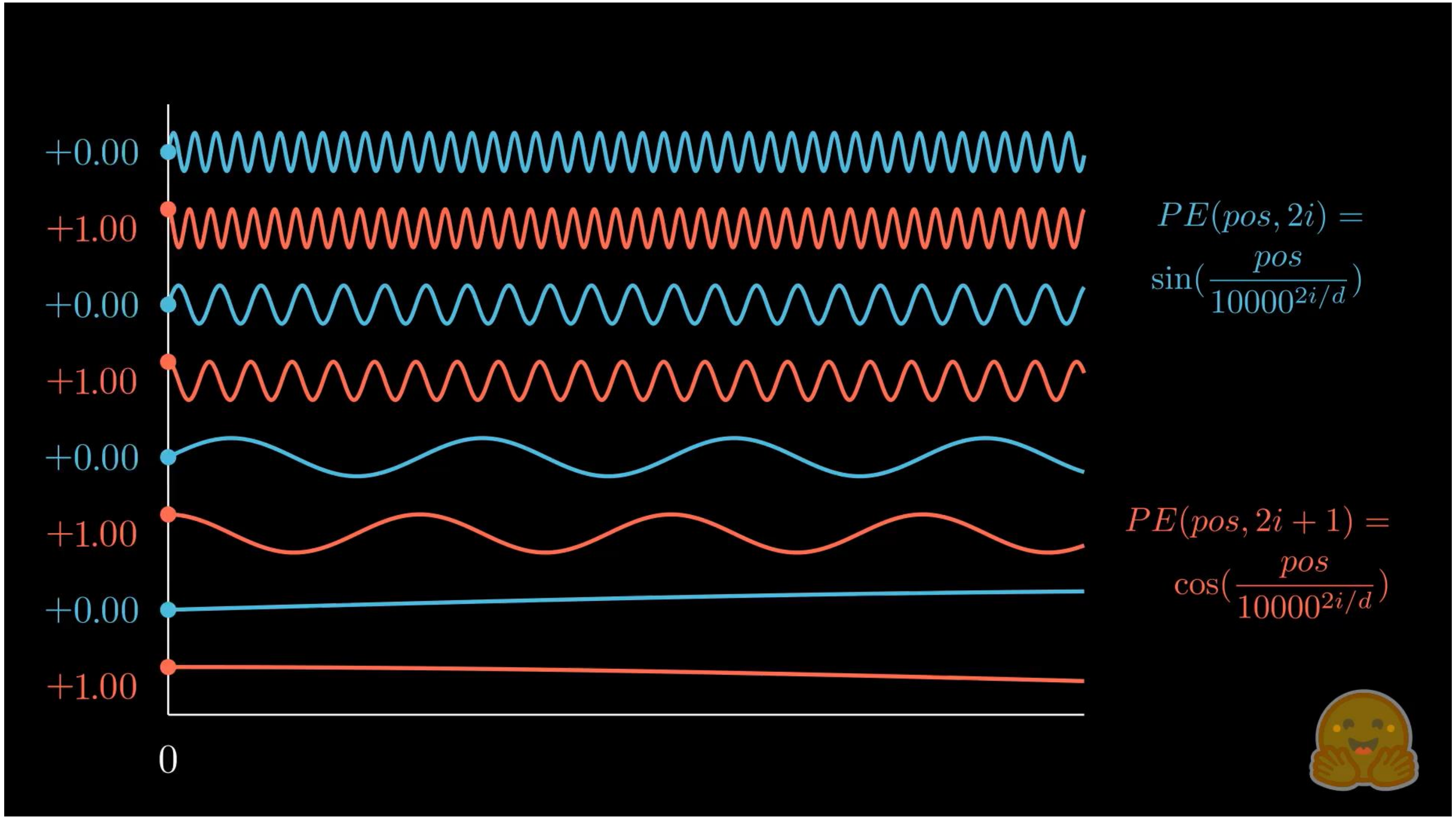

$$PE(pos, 2i) = \sin\left(\frac{pos}{10000^{\frac{2i}{d}}}\right)$$

$$PE(pos, 2i+1) = \cos\left(\frac{pos}{10000^{\frac{2i}{d}}}\right)$$

Encoding word positions

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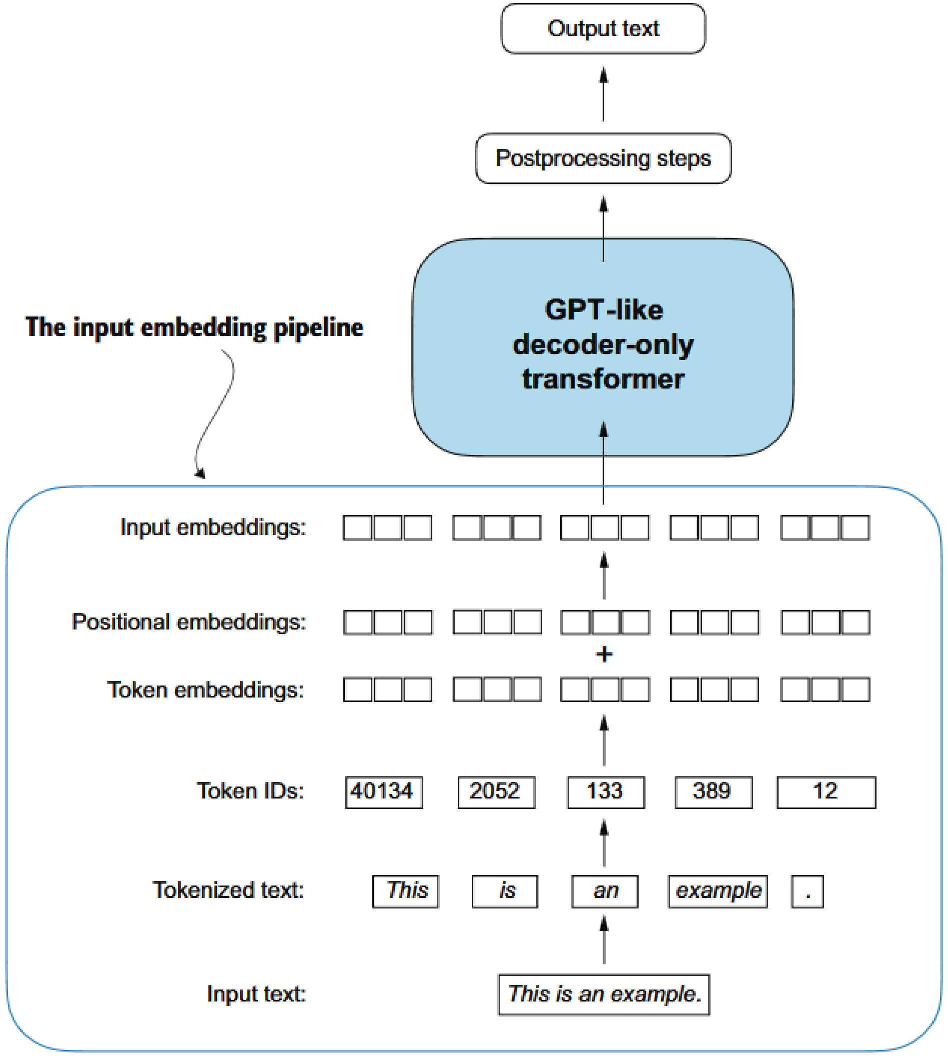
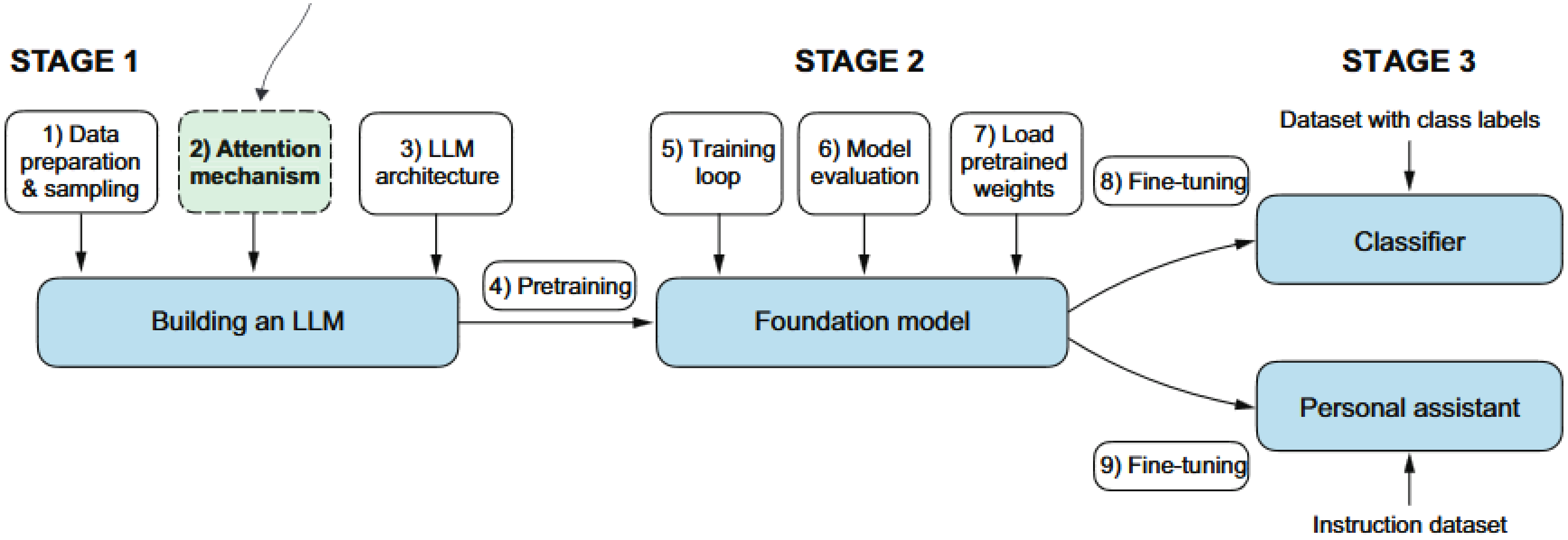
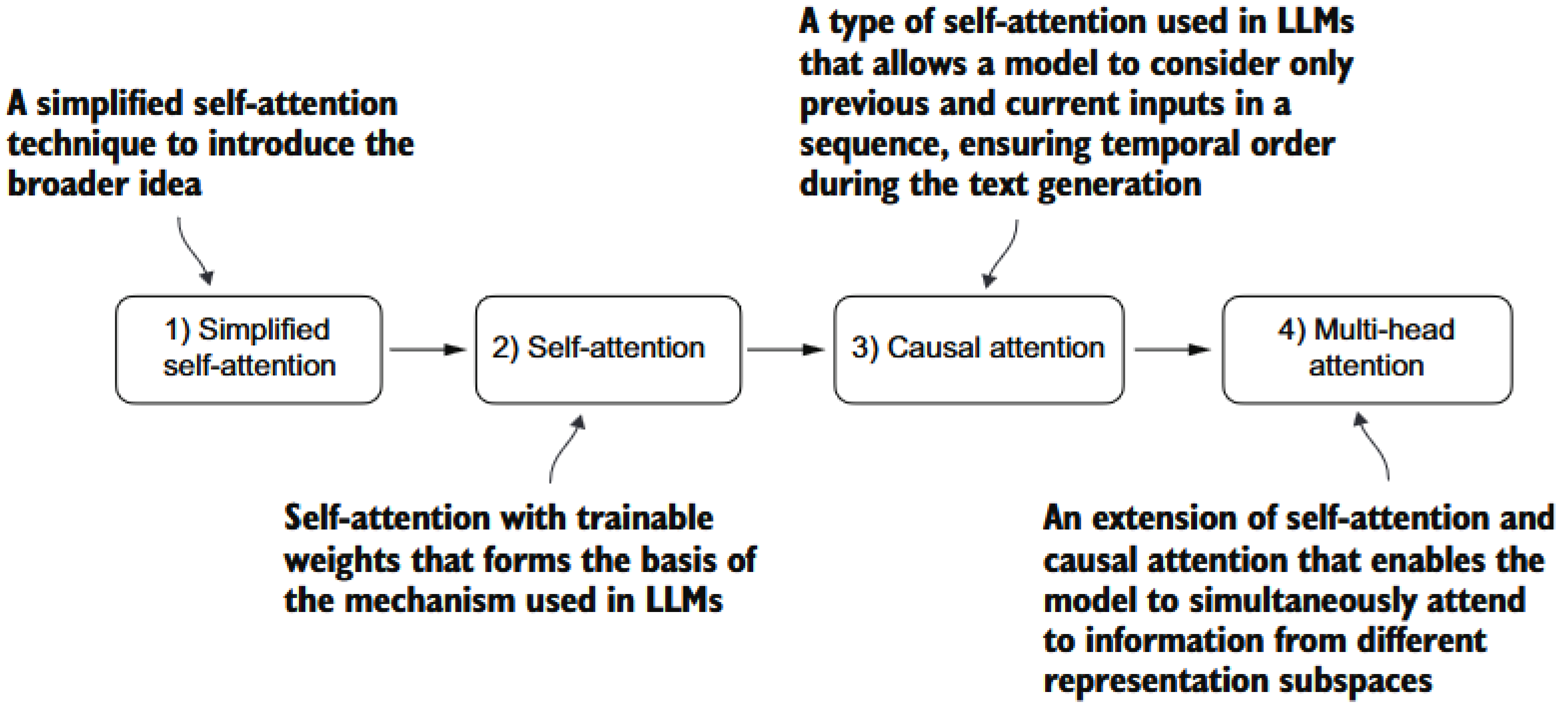


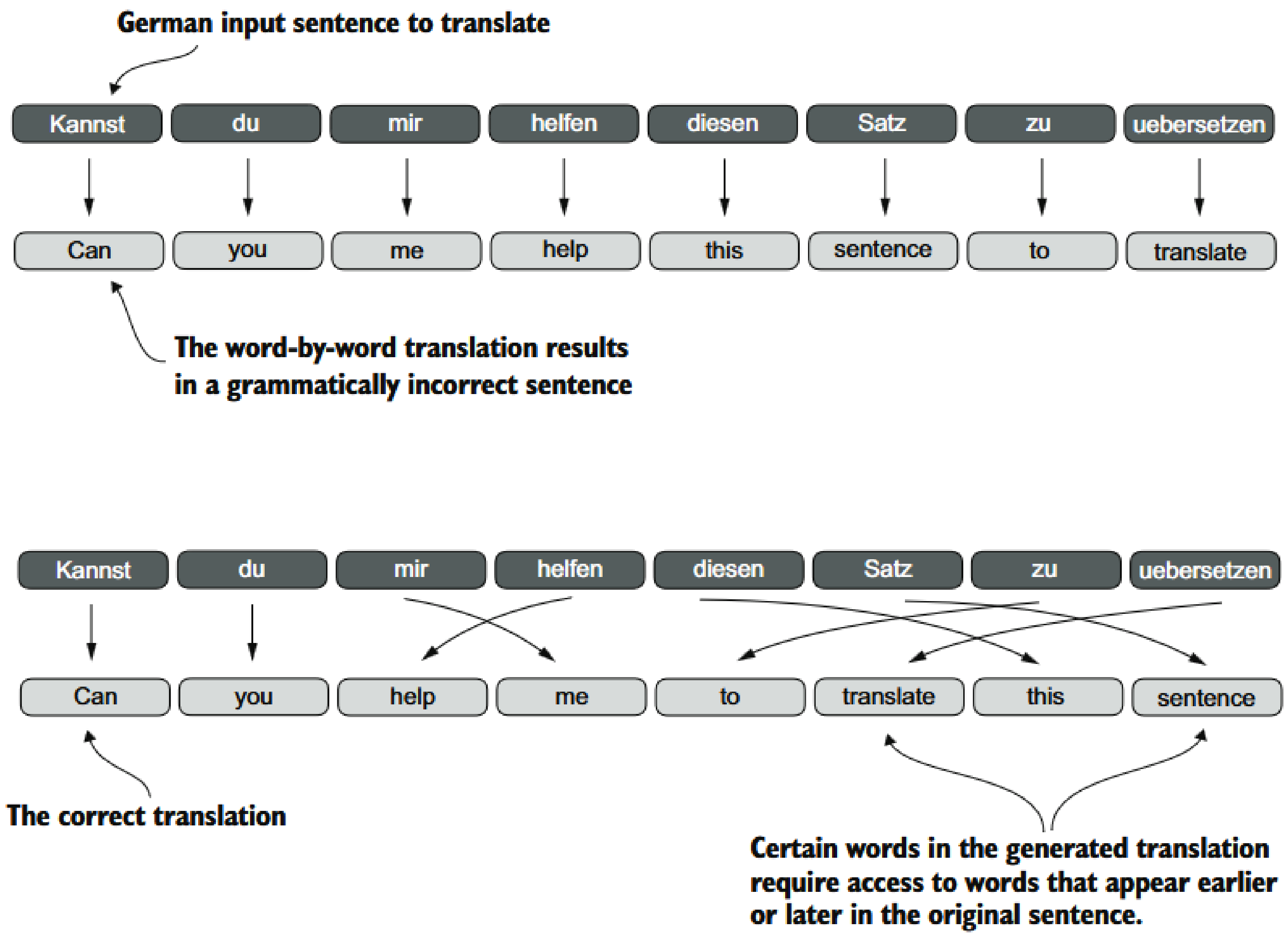
Attention mechanism



Attention mechanism



Problem with modeling long sequences



Modeling sequences

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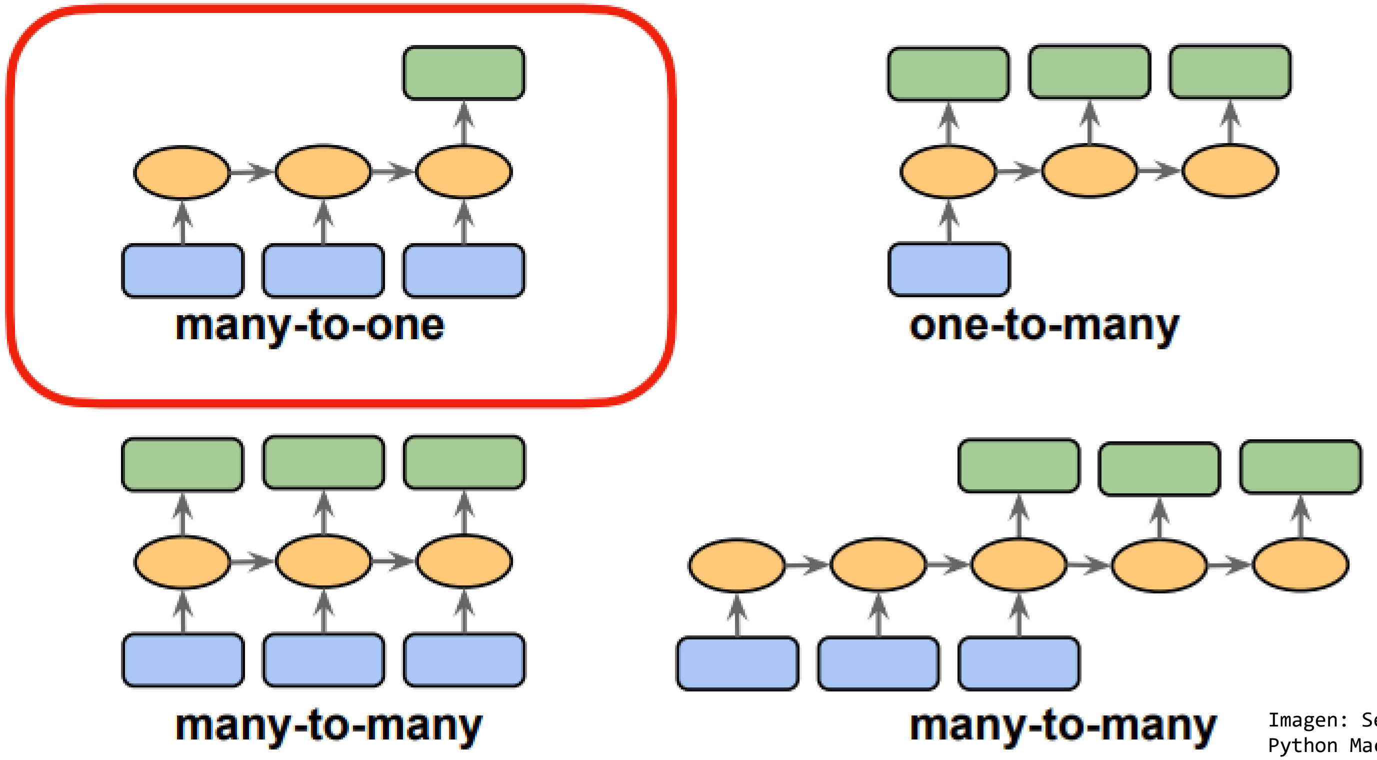
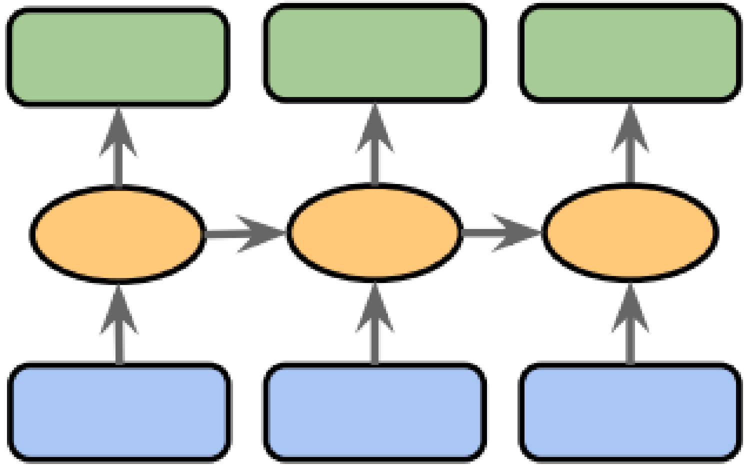


Imagen: Sebastian Raschka, Vahid Mirjalili.
Python Machine Learning. 3rd Edition.
Birmingham, UK: Packt Publishing, 2019

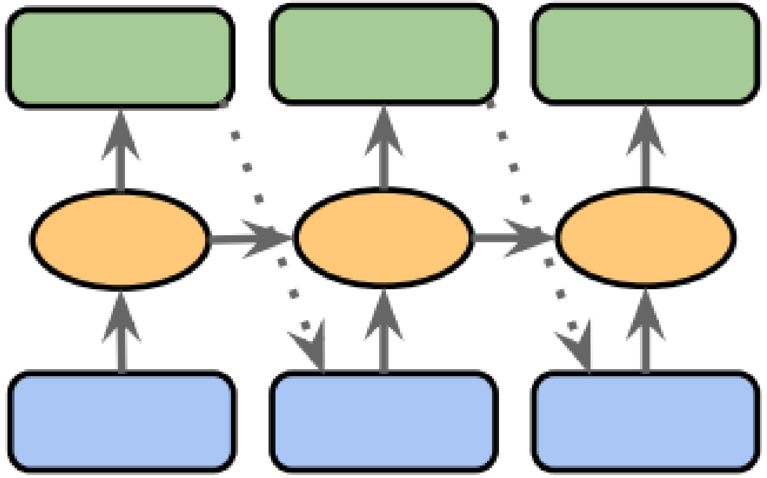
The Unreasonable Effectiveness of Recurrent Neural Networks by Andrej Karpathy (http://karpathy.github.io/2015/05/21/rnn-effectiveness/)

Modeling sequences



many-to-many

"training"

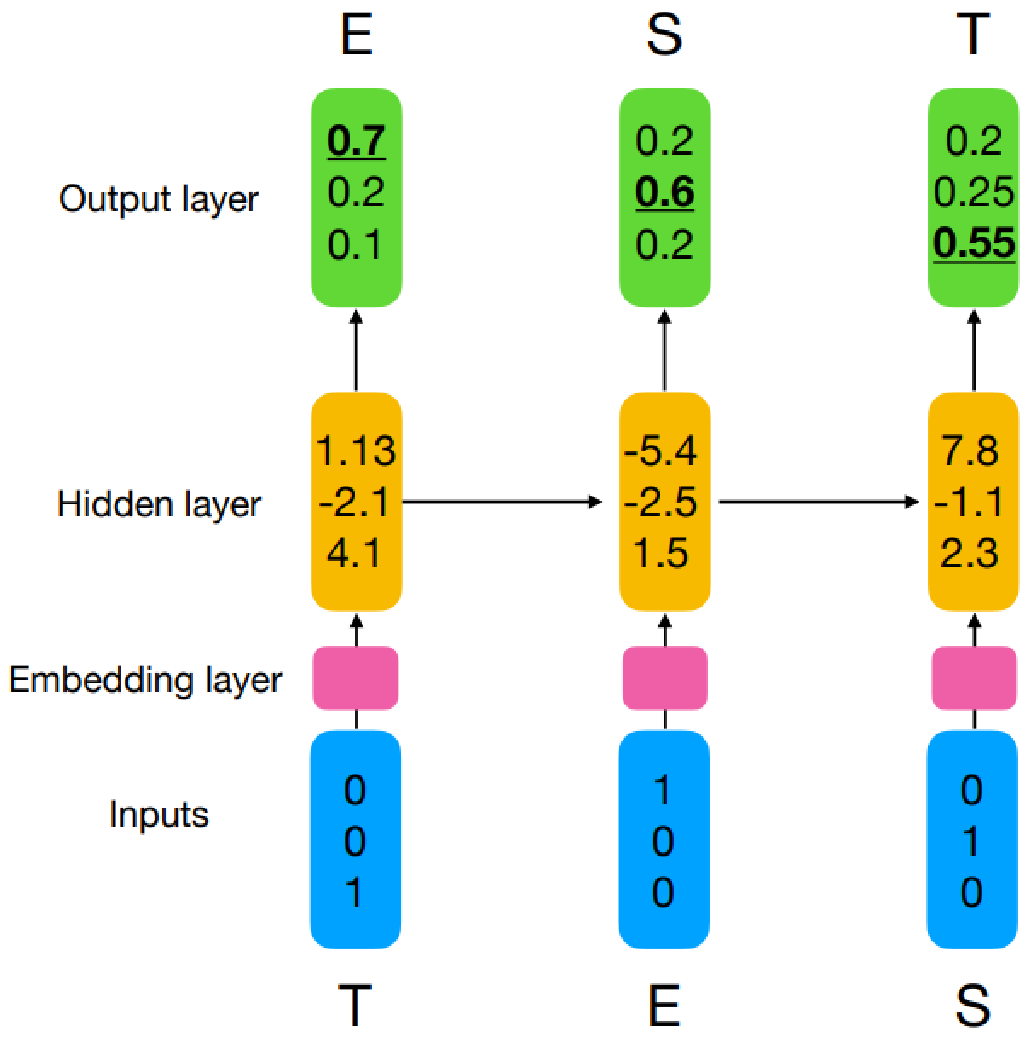


~~many~~-to-many

"one"

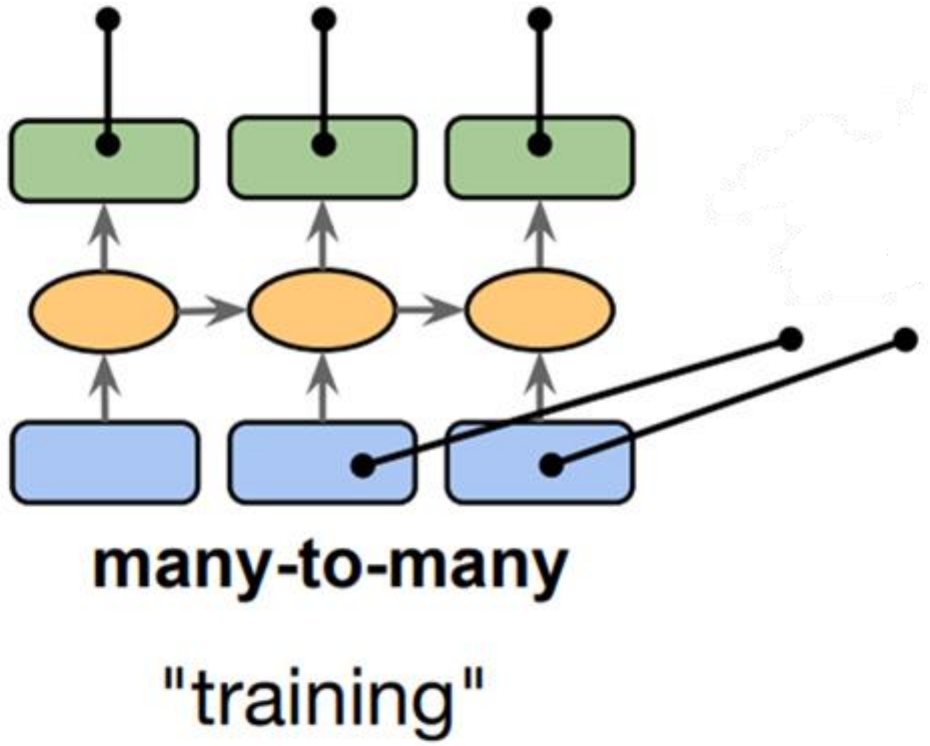
"generating new text"

Recurrent Neural Networks



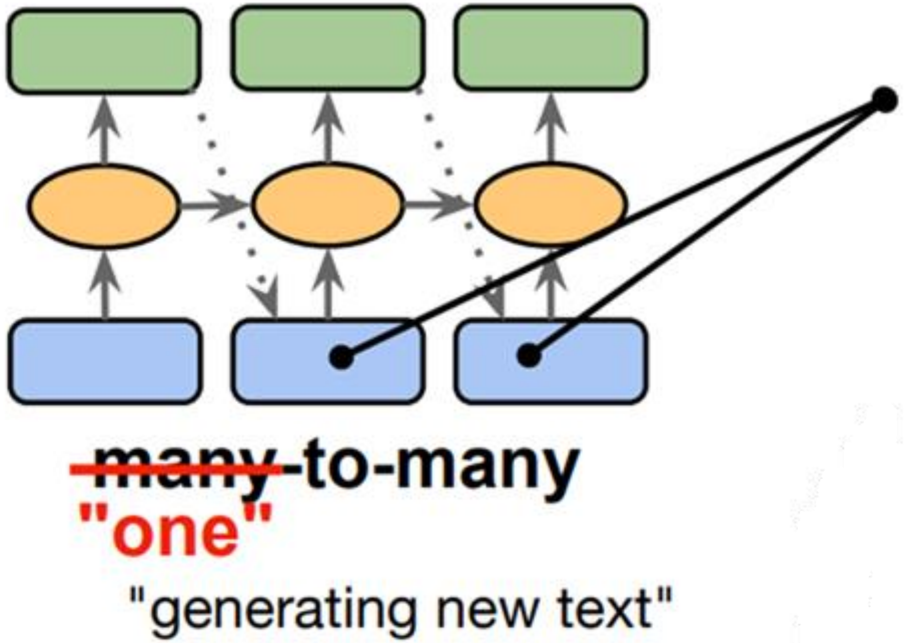
Recurrent Neural Networks

At each time step, Softmax output (probability) for each possible 'next letter



For the next input, ignore the prediction but use the 'correct' next letter from the dataset.

Recurrent Neural Networks



To generate new text, now display the softmax outputs and provide the letter as input for the next time step.

Long Short Term Memory Networks

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https://pytorch.org/docs/stable/generated/torch.nn.LSTM.html

Parameters

- **input_size** – The number of expected features in the input *x*
- **hidden_size** – The number of features in the hidden state *h*
- **num_layers** – Number of recurrent layers. E.g., setting `num_layers=2` would mean stacking two LSTMs together to form a *stacked LSTM*, with the second LSTM taking in outputs of the first LSTM and computing the final results. Default: 1
- **bias** – If `False`, then the layer does not use bias weights *b_ih* and *b_hh*. Default: `True`
- **batch_first** – If `True`, then the input and output tensors are provided as (batch, seq, feature). Default: `False`
- **dropout** – If non-zero, introduces a *Dropout* layer on the outputs of each LSTM layer except the last layer, with dropout probability equal to `dropout`. Default: 0
- **bidirectional** – If `True`, becomes a bidirectional LSTM. Default: `False`
- **proj_size** – If `> 0`, will use LSTM with projections of corresponding size. Default: 0

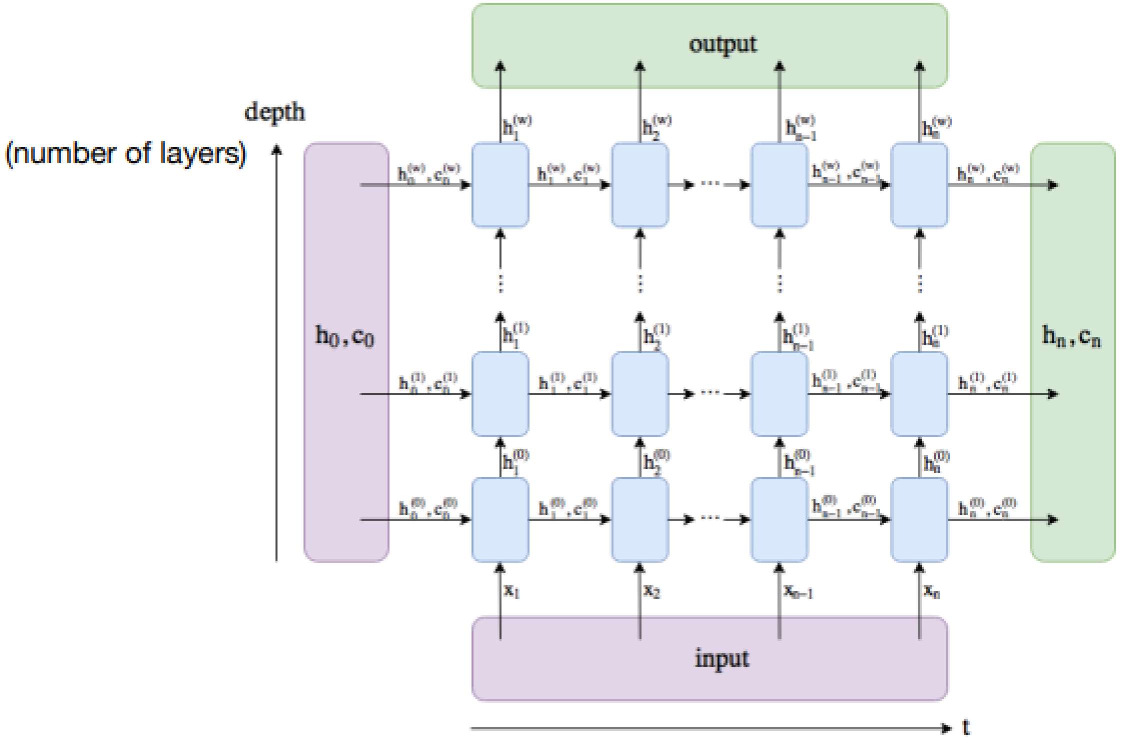
Examples:

```
>>> rnn = nn.LSTM(10, 20, 2)
>>> input = torch.randn(5, 3, 10)
>>> h0 = torch.randn(2, 3, 20)
>>> c0 = torch.randn(2, 3, 20)
>>> output, (hn, cn) = rnn(input, (h0, c0))
```

LSTM

Examples:

```
>>> rnn = nn.LSTM(10, 20, 2)
>>> input = torch.randn(5, 3, 10)
>>> h0 = torch.randn(2, 3, 20)
>>> c0 = torch.randn(2, 3, 20)
>>> output, (hn, cn) = rnn(input, (h0, c0))
```



Fuente de imagen: https://stackoverflow.com/questions/48302810/whats-the-difference-between-hidden-and-output-in-pytorch-lstm

LSTM

https://pytorch.org/docs/stable/generated/torch.nn.LSTMCell.html

Inputs: input, (h_0, c_0)

- **input** of shape (*batch*, *input_size*): tensor containing input features
- **h_0** of shape (*batch*, *hidden_size*): tensor containing the initial hidden state for each element in the batch.
- **c_0** of shape (*batch*, *hidden_size*): tensor containing the initial cell state for each element in the batch.

  If (*h_0*, *c_0*) is not provided, both **h_0** and **c_0** default to zero.

Outputs: (h_1, c_1)

- **h_1** of shape (*batch*, *hidden_size*): tensor containing the next hidden state for each element in the batch
- **c_1** of shape (*batch*, *hidden_size*): tensor containing the next cell state for each element in the batch

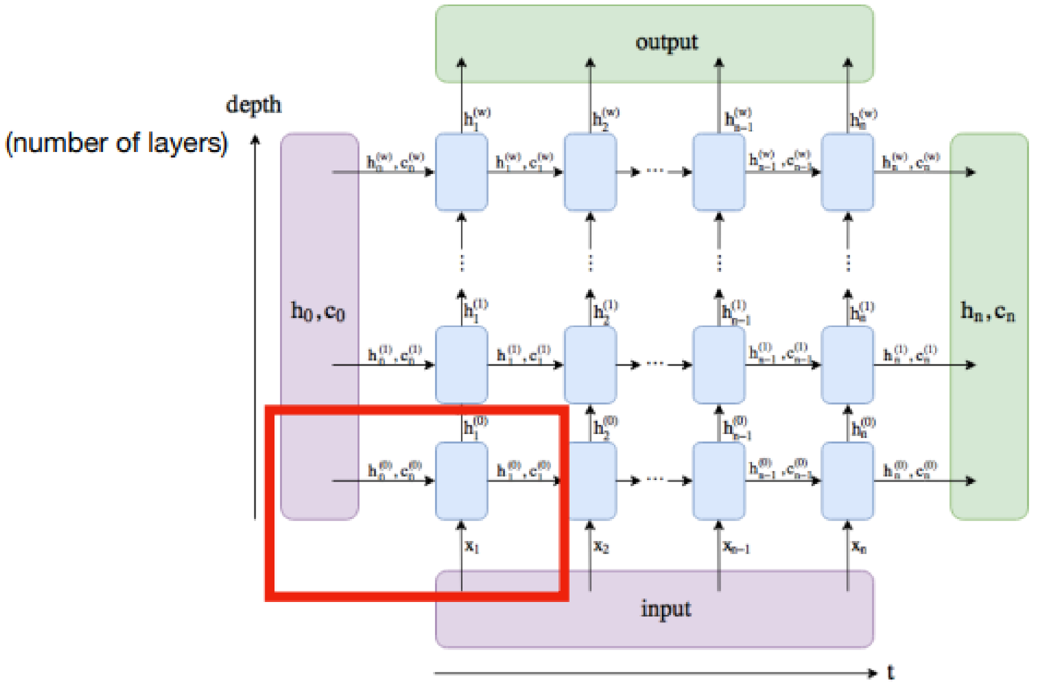
Examples:

```
>>> rnn = nn.LSTMCell(10, 20) # (input_size, hidden_size)
>>> input = torch.randn(2, 3, 10) # (time_steps, batch, input_size)
>>> hx = torch.randn(3, 20) # (batch, hidden_size)
>>> cx = torch.randn(3, 20)
>>> output = []
>>> for i in range(input.size()[0]):
        hx, cx = rnn(input[i], (hx, cx))
        output.append(hx)
>>> output = torch.stack(output, dim=0)
```

Clase LSTM

Examples:

```
>>> rnn = nn.LSTMCell(10, 20) # (input_size, hidden_size)
>>> input = torch.randn(2, 3, 10) # (time_steps, batch, input_size)
>>> hx = torch.randn(3, 20) # (batch, hidden_size)
>>> cx = torch.randn(3, 20)
>>> output = []
>>> for i in range(input.size()[0]):
        hx, cx = rnn(input[i], (hx, cx))
        output.append(hx)
>>> output = torch.stack(output, dim=0)
```



Fuente de imagen: https://stackoverflow.com/questions/48302810/whats-the-difference-between-hidden-and-output-in-pytorch-lstm

Seq2seq

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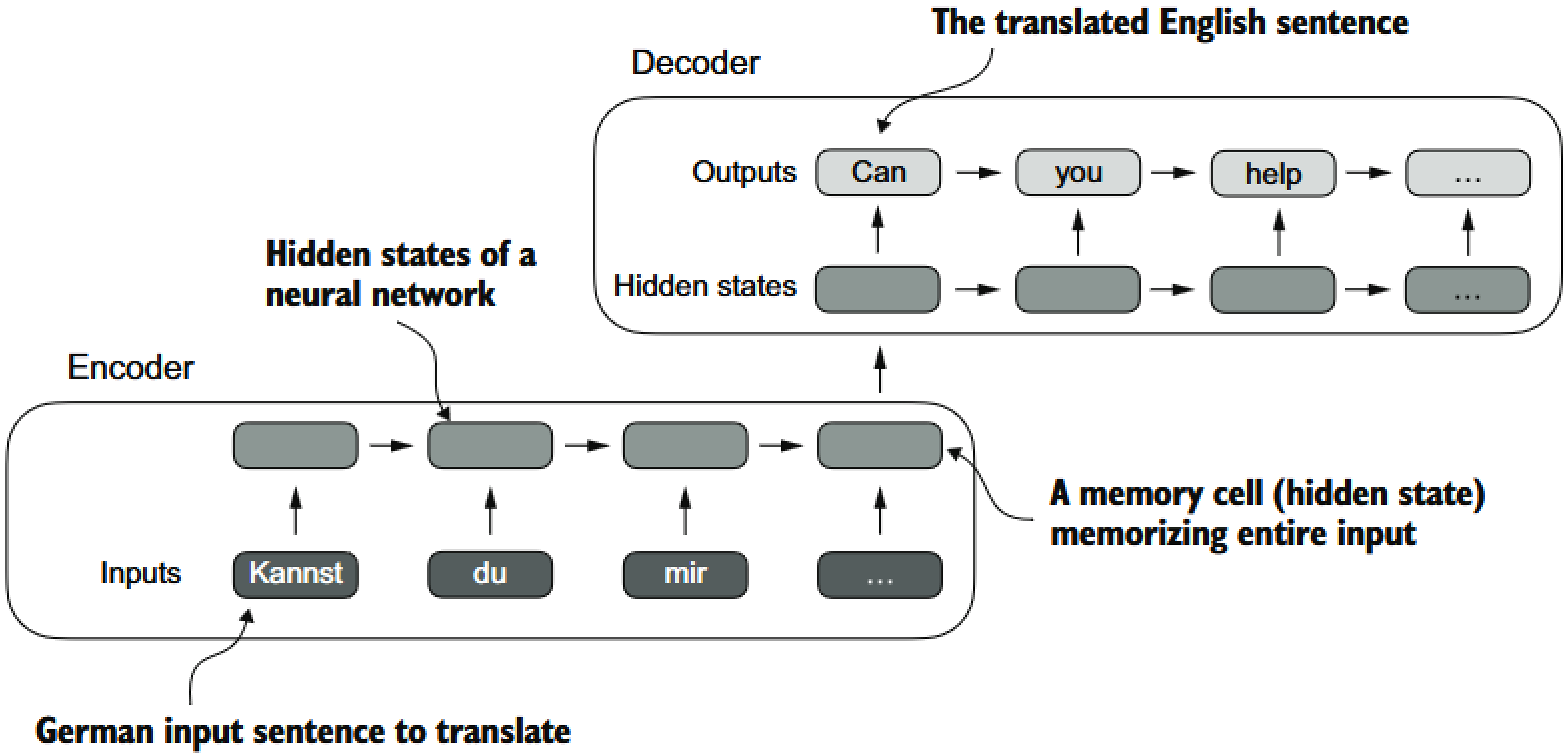

Attention mechanism

Assign an attention weight to each word to determine how much 'attention' the model should pay to each word (that is, for each word, the network learns a 'context').

Attention mechanism

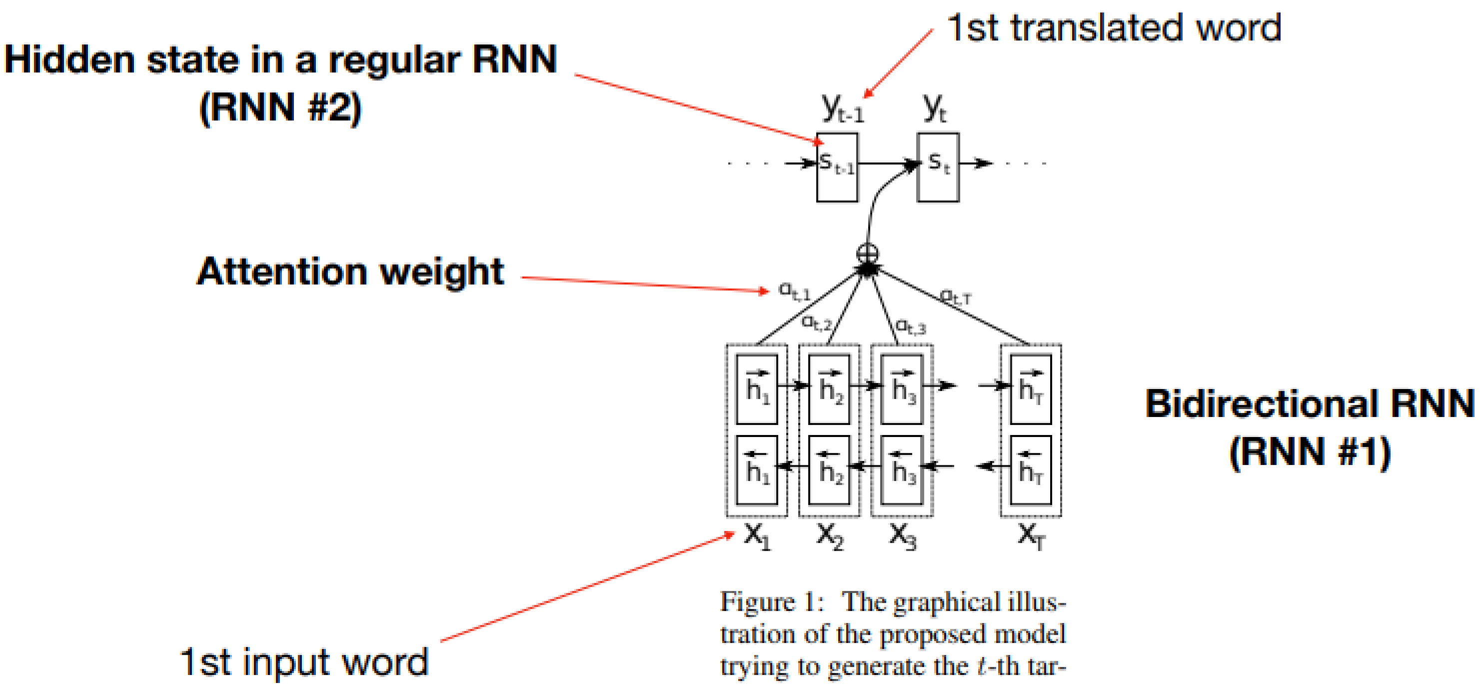

Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

NEURAL MACHINE TRANSLATION
BY JOINTLY LEARNING TO ALIGN AND TRANSLATE

Dzmitry Bahdanau
Jacobs University Bremen, Germany

KyungHyun Cho **Yoshua Bengio***
Université de Montréal

ABSTRACT

Attention is all you need

Attention Is All You Need

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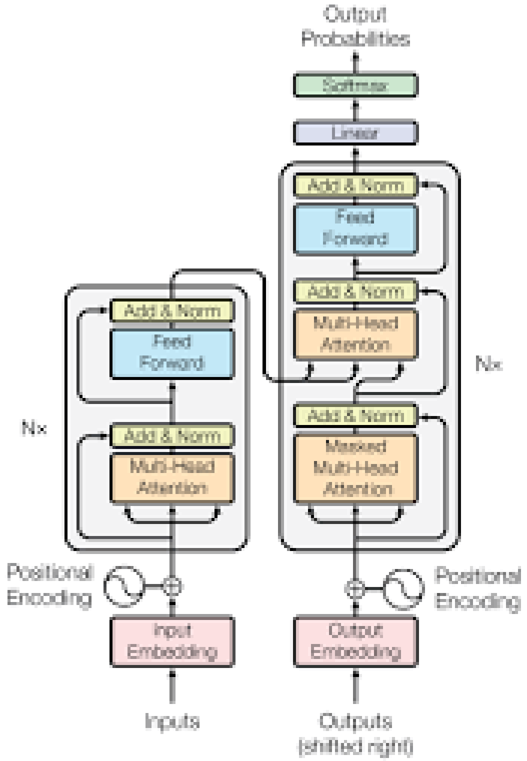

Since ~2018, transformers have been growing in popularity... and size

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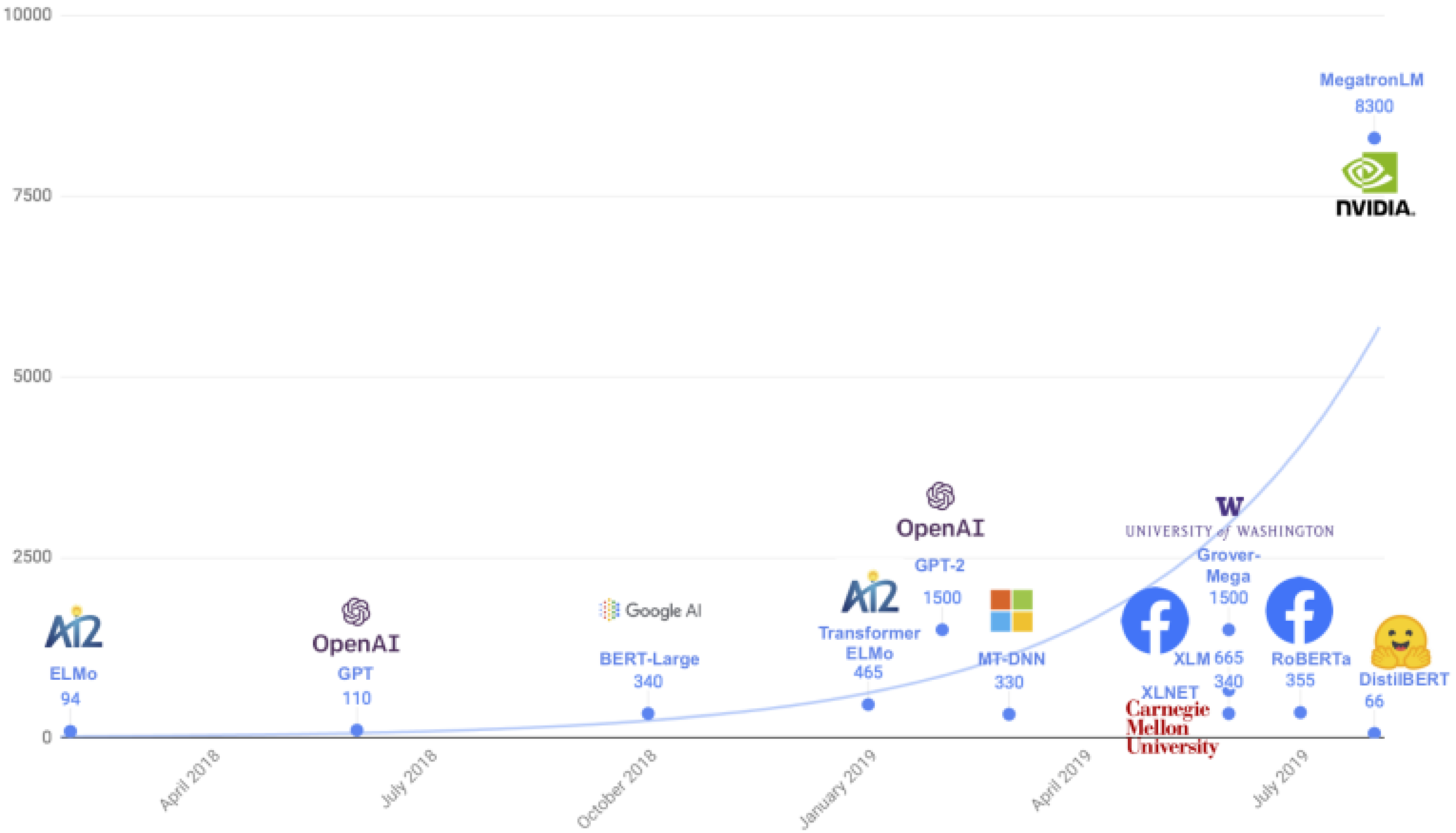
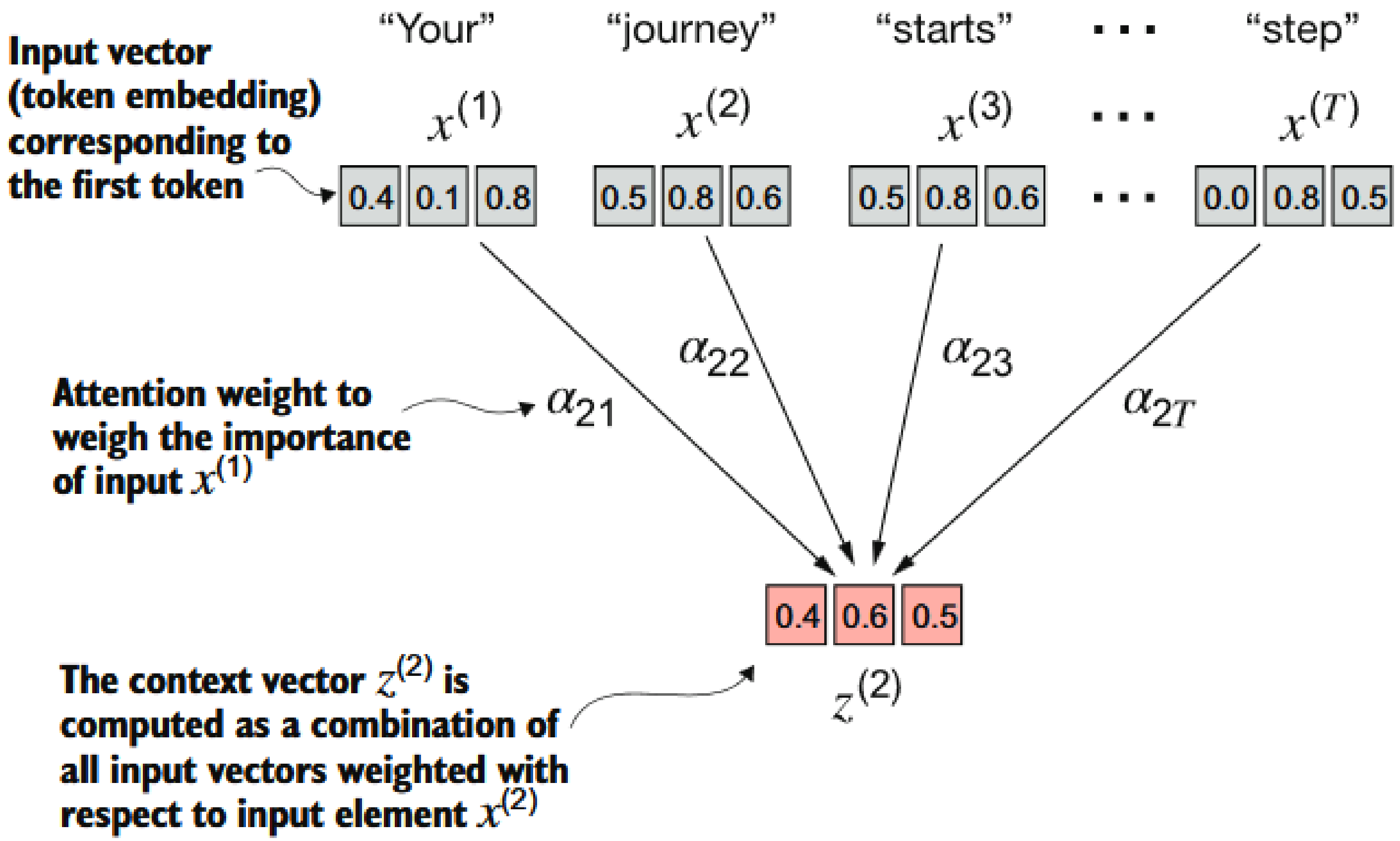


Fuente imagen: https://medium.com/huggingface/distilbert-8cf3380435b5

A simple self-attention mechanism without trainable weights



A simple self-attention mechanism without trainable weights

Self-attention as weighted sum:

$$A_i = \sum_{j=0}^{T} a_{ij} x_j$$

output corresponding to the i-th input

weight based on similarity between current input x_i and all other inputs

How to compute the attention weights?

here as simple dot product:

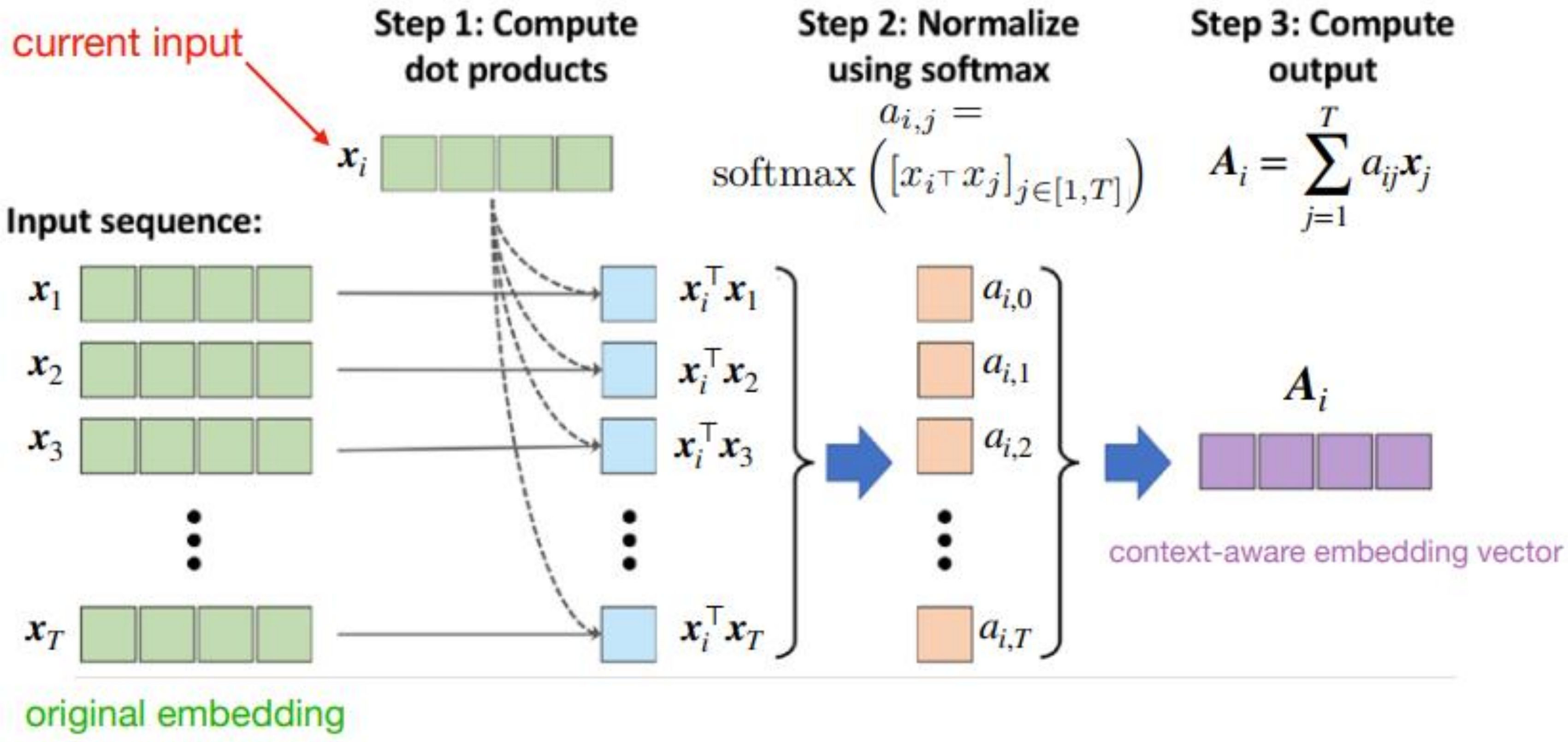
$$e_{ij} = x_i^{\top} x_j$$

repeat this for all inputs $j \in \{1 \ldots T\}$, then normalize

$$a_{ij} = \frac{\exp\left(e_{ij}\right)}{\sum_{j=1}^{T} \exp\left(e_{ij}\right)} = \text{softmax}\left(\left[e_{ij}\right]_{j=1 \ldots T}\right)$$

A simple self-attention mechanism without trainable weights

Self-attention: Relating different positions within a single sequence (vs. between input and output sequences



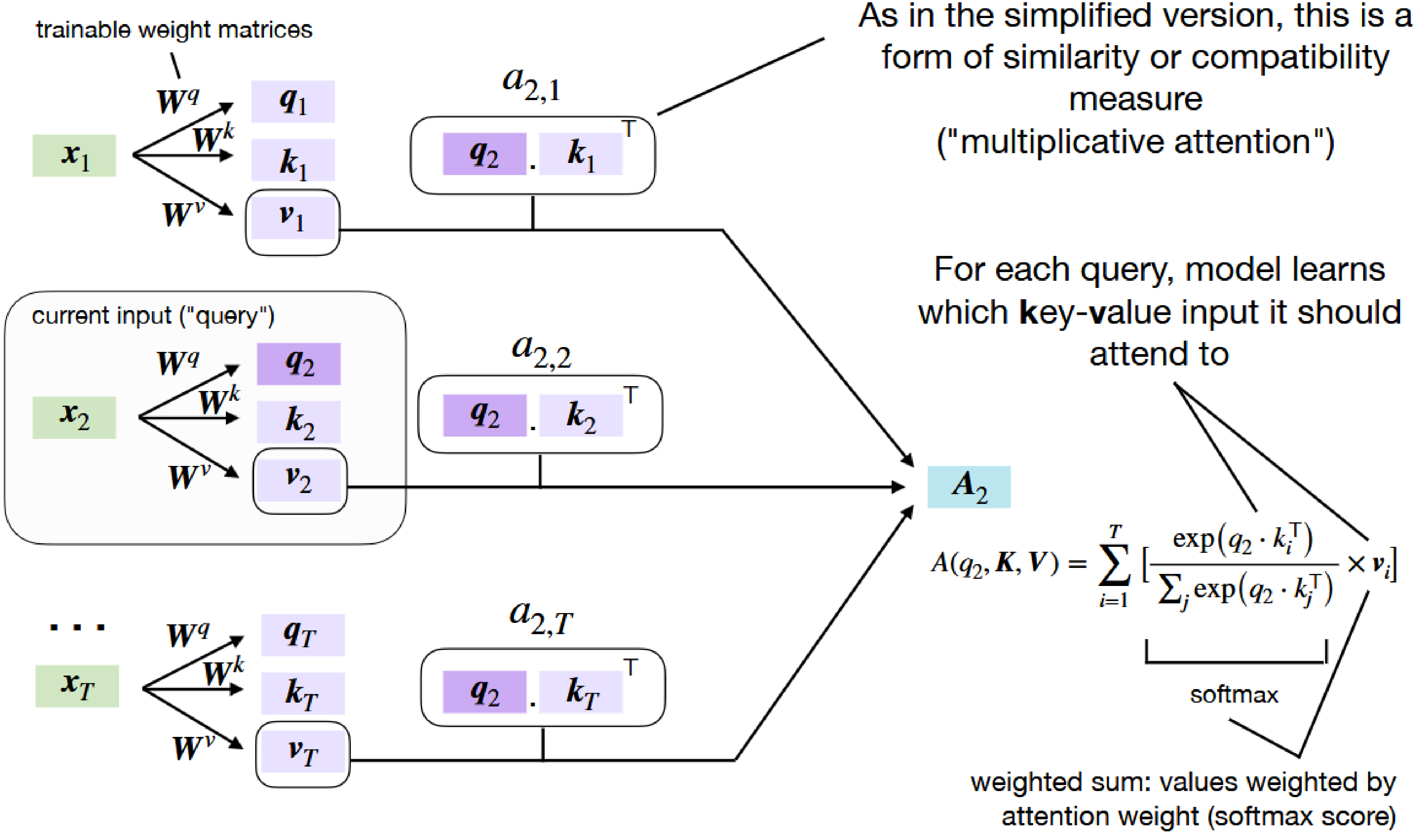
Raschka & Mirjalili 2019. Python Machine Learning, 3rd edition

Self-attention mechanism

- Previous basic version did not involve any learnable parameters, so not very useful for learning a language model
- We are now adding 3 trainable weight matrices that are multiplied with the input sequence embeddings

$$\text{query} = \boldsymbol{W}^q \boldsymbol{x}_i$$
$$\text{key} = \boldsymbol{W}^k \boldsymbol{x}_i$$
$$\text{value} = \boldsymbol{W}^v \boldsymbol{x}_i$$

Self-attention mechanism



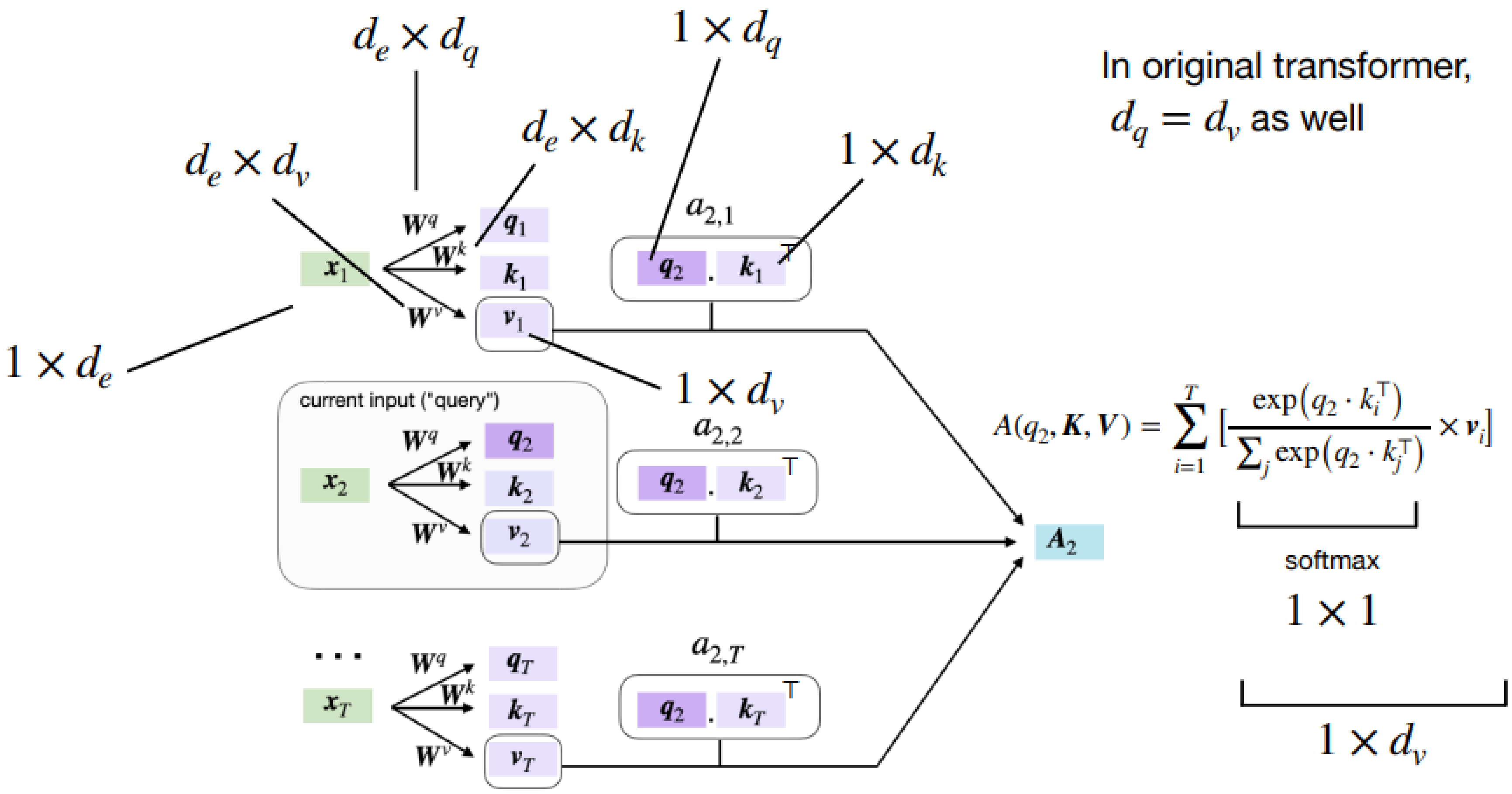
$$A(q_2, \boldsymbol{K}, \boldsymbol{V}) = \sum_{i=1}^{T} \Big[\underbrace{\frac{\exp(q_2 \cdot k_i^{\top})}{\sum_j \exp(q_2 \cdot k_j^{\top})}}_{\text{softmax}} \times \boldsymbol{v}_i\Big]$$

Self-attention mechanism

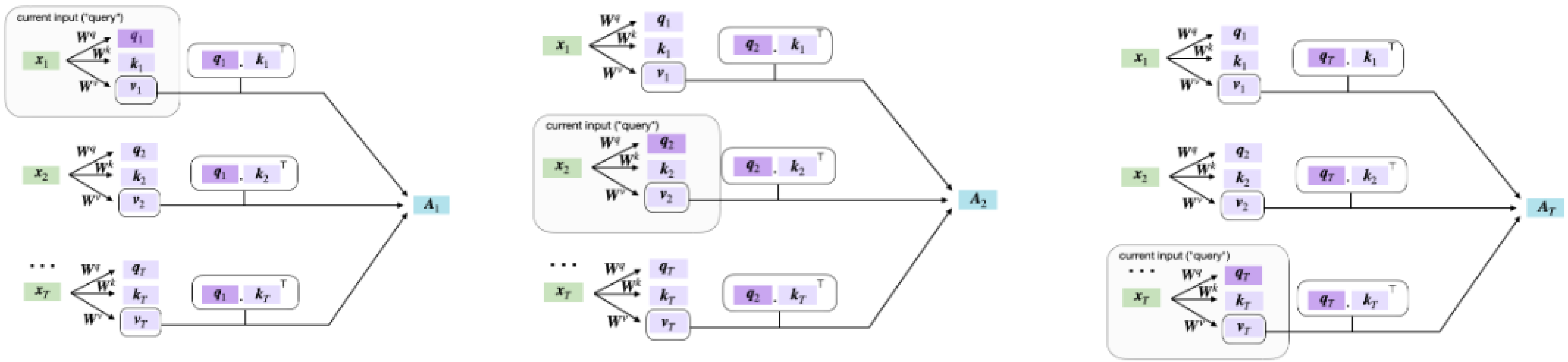
d_e = embedding size (original transformer = 512)

where $d_q = d_k$

In original transformer, $d_q = d_v$ as well



Self-attention mechanism



Attention score matrix: $A = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix}$

Self attention mechanism – Scaled dot producto attention

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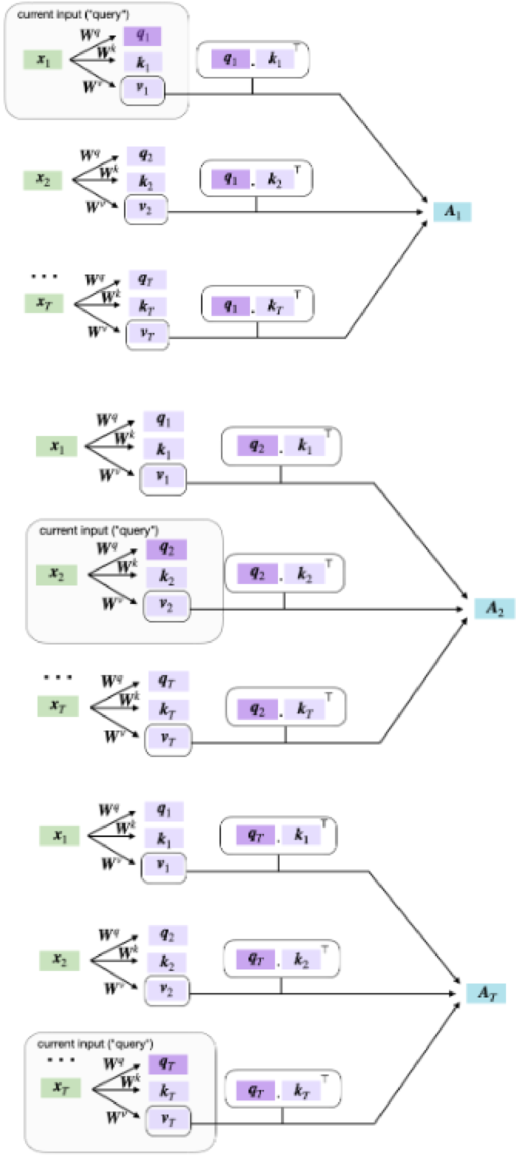
d_e = embedding size

T = input sequence size

$$\boldsymbol{x} \in \mathbb{R}^{T \times d_e}$$



$$\boldsymbol{Q} \in \mathbb{R}^{T \times d_q}$$

$$\boldsymbol{K} \in \mathbb{R}^{T \times d_k}$$

$$\boldsymbol{V} \in \mathbb{R}^{T \times d_v}$$

$$\underbrace{A(Q,K,V) = \overbrace{\text{softmax}\left(\frac{QK^{\top}}{\sqrt{d_k}}\right)}^{\substack{\text{"attention matrix"} \\ T \times T}} \boldsymbol{V}}_{\substack{T \times d_v \\ \text{"attention-based embedding"}}}$$

Scaled dot product attention

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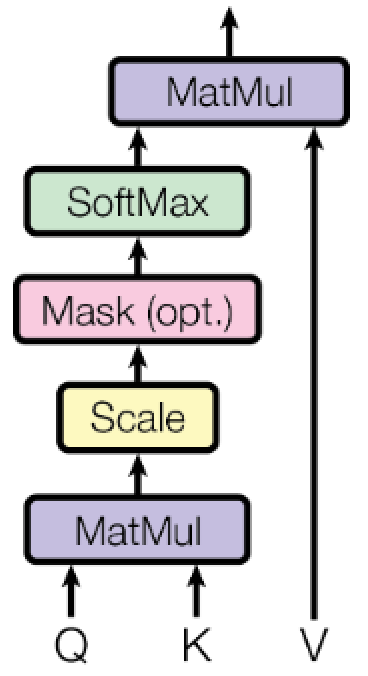
$$A(Q, K, V) = \text{softmax}\left(\frac{QK^{\top}}{\sqrt{d_k}}\right)V$$

To ensure that the dot-products between query and and key don't grow too large (and softmax gradient become too small) for large d_k

Scaled Dot-Product Attention



Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Multi-Head attention

- Apply self-attention multiple times in parallel (similar to multiple kernels for channels in CNNs)

- For each head (self-attention layer), use different $\mathbf{W}^{q}, \mathbf{W}^{k}, \mathbf{W}^{v}$ then concatenate the results $\mathbf{A}_{(i)}$.

- 8 attention heads in the original transformer.

- Allows attending to different parts in the sequence differently.

Multi-Head attention

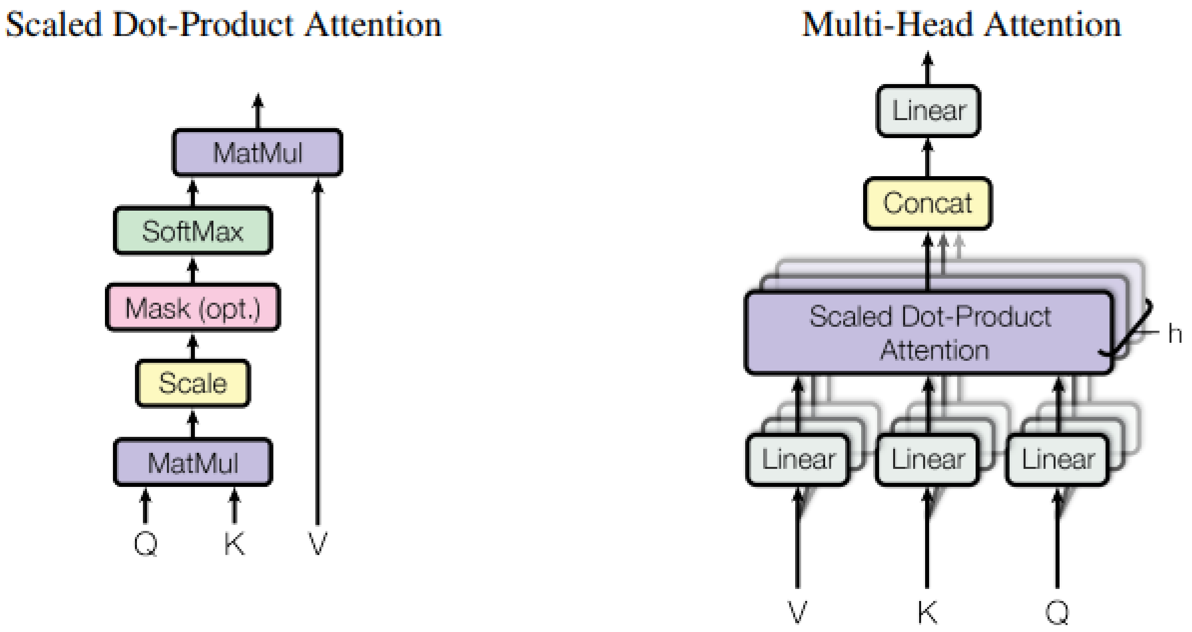
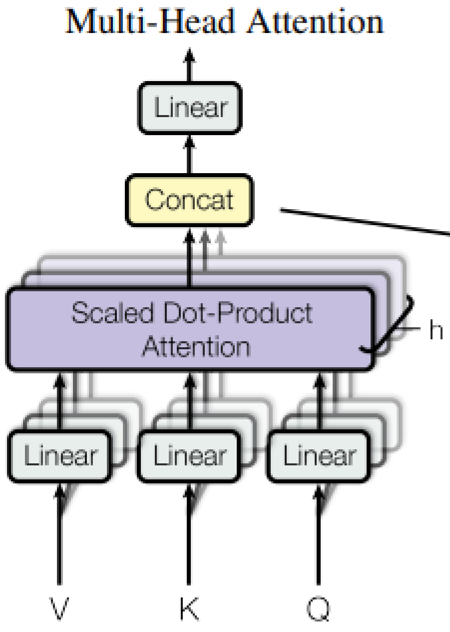
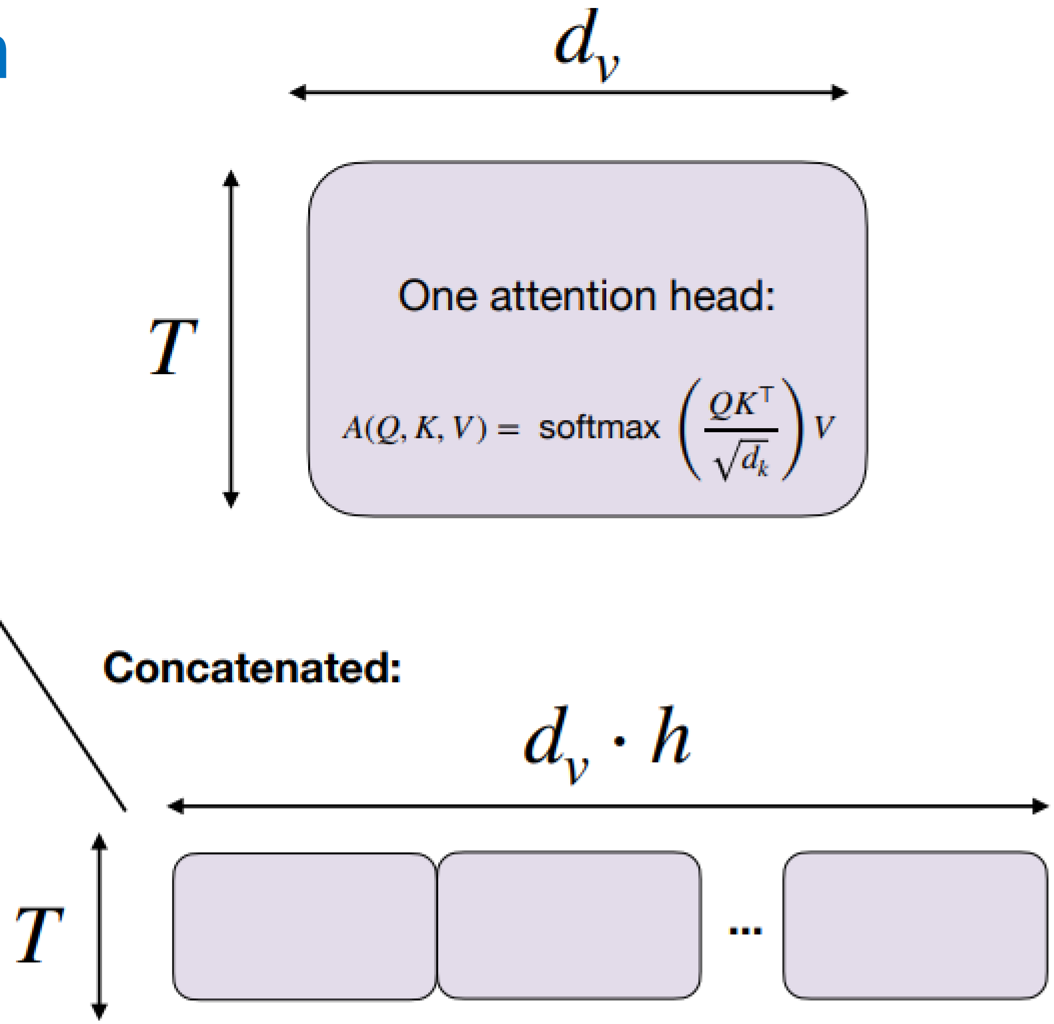


Figure 2: (left) Scaled Dot-Product Attention. (right) Multi-Head Attention consists of several attention layers running in parallel.

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Multi-Head attention





Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

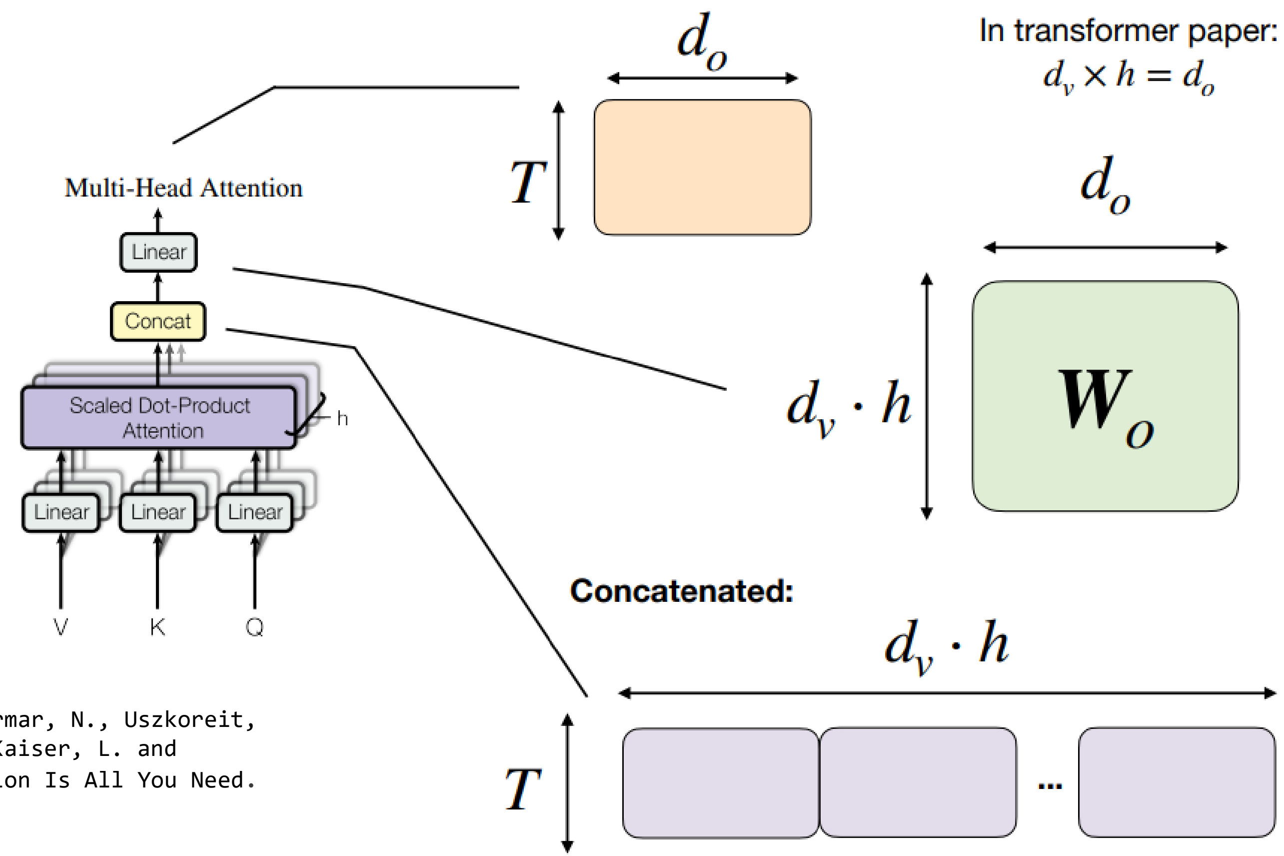
Dimensión de la sequencia de entrada en el transformador orginal:

$$T \times d_e = T \times 512$$

y

$$d_v = 512/h = 64$$

Multi-Head attention



Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Scaled Dot-Product Attention Recap

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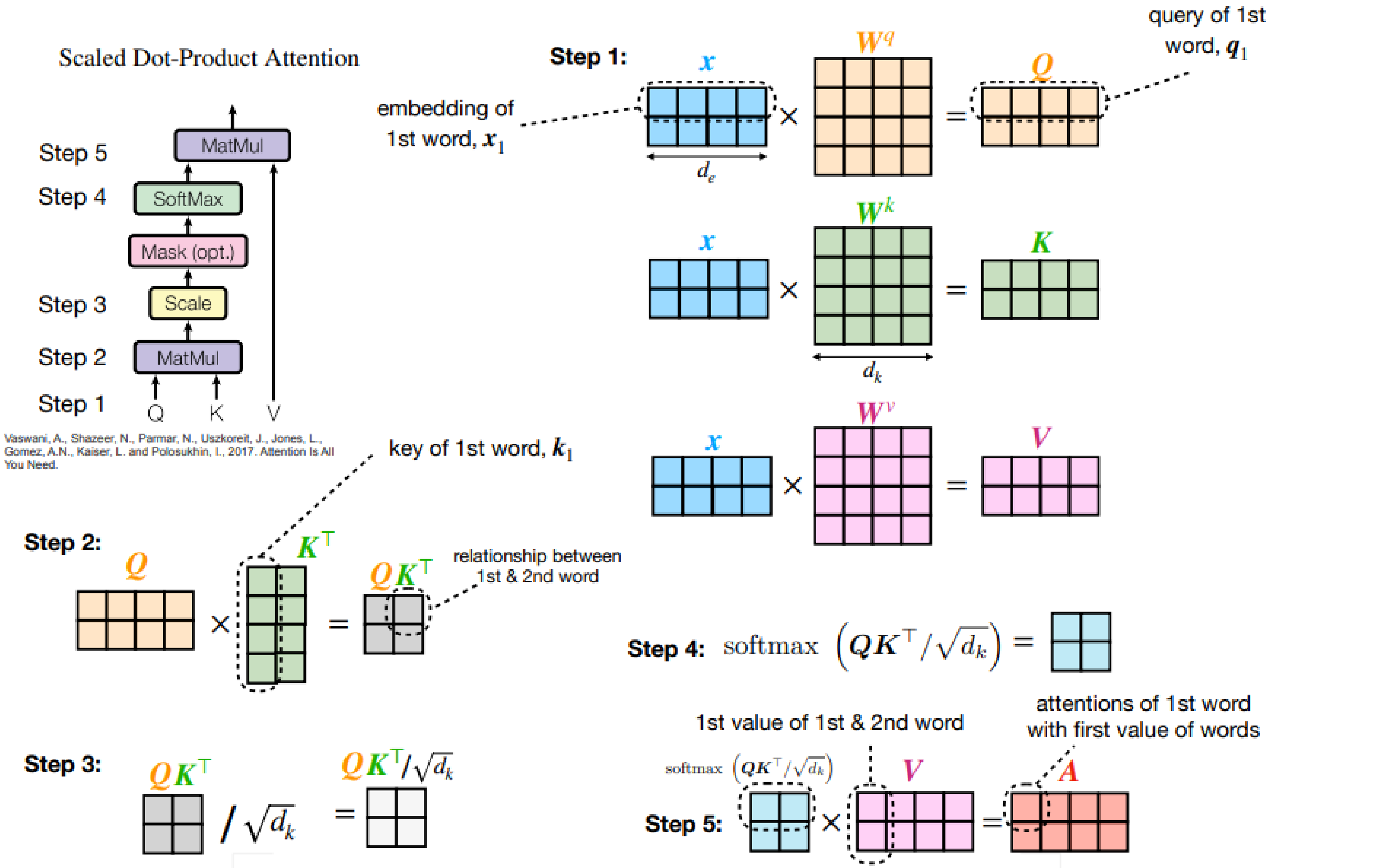

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Scaled Dot-Product Attention Recap

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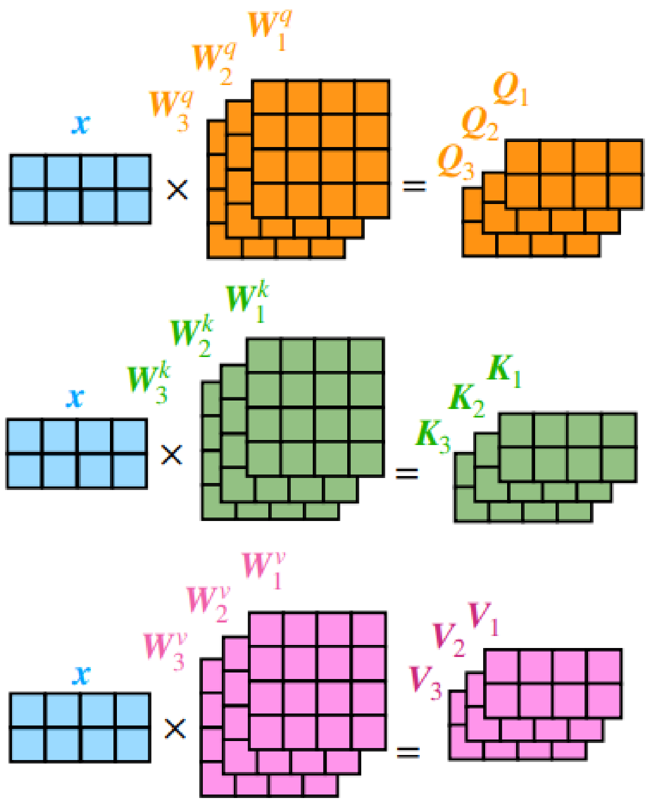

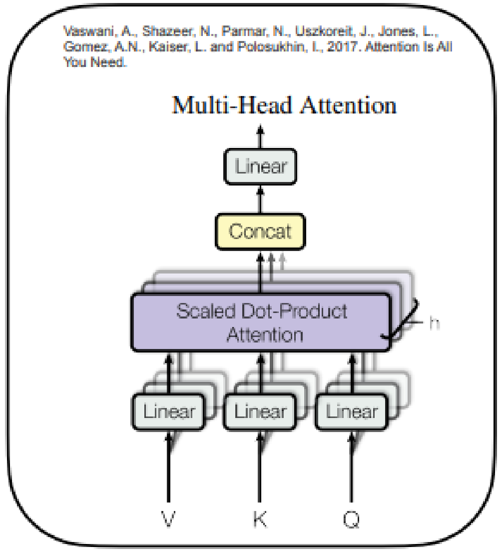

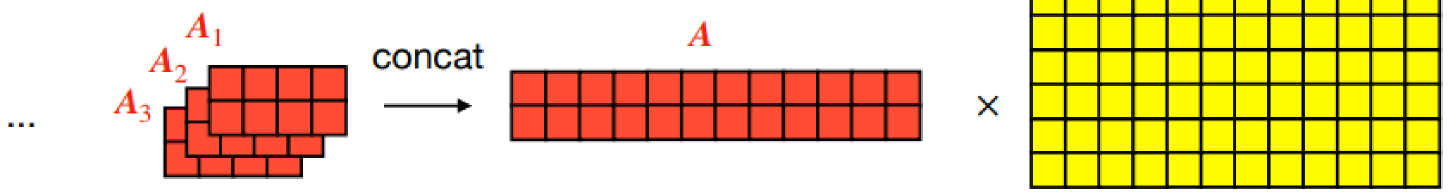

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Recommended reading

https://jalammar.github.io/illustrated-transformer/