Transformers

Course Instructor: Chandresh
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Course Content

Module I: History of Deep Learning, Sigmoid Neurons, Perceptrons, and learning algorithms. Multilayer Perceptrons (MLPs), Representation Power of MLPs,.

Module II: Feedforward Neural Networks. Backpropagation. first and second-order training methods. NN Training tricks, Regularization

Module III: Introduction to Autoencoders and their characteristics, relation to PCA, Regularization in autoencoders, and Types of autoencoders, Variational Autoencoder

Module IV: Architecture of Convolutional Neural Networks (CNN), types of CNNs. Image classification, Pre-training vs fine-tuning.- representation learning, Object Detection and Semantic Segmentation

Module V: Architecture of Recurrent Neural Networks (RNN), Word Embeddings,
Encoder-Decoder Models, Attention Mechanism. Advanced Topics: **Transformers** and BERT. Nodule VI: Gen AI- Deep generative models: VAE, GAN,

Acknowledgement

- Russ Salakhutdinov and Hugo Larochelle's class on Neural Networks
- Neural Networks and Deep Learning course by Danna Gurari University of Colorado Boulder

Today’s Topics

- Transformer overview
- Self-attention
- Multi-head attention
- Common transformer ingredients
- Pioneering transformer: machine translation
- Programming tutorial

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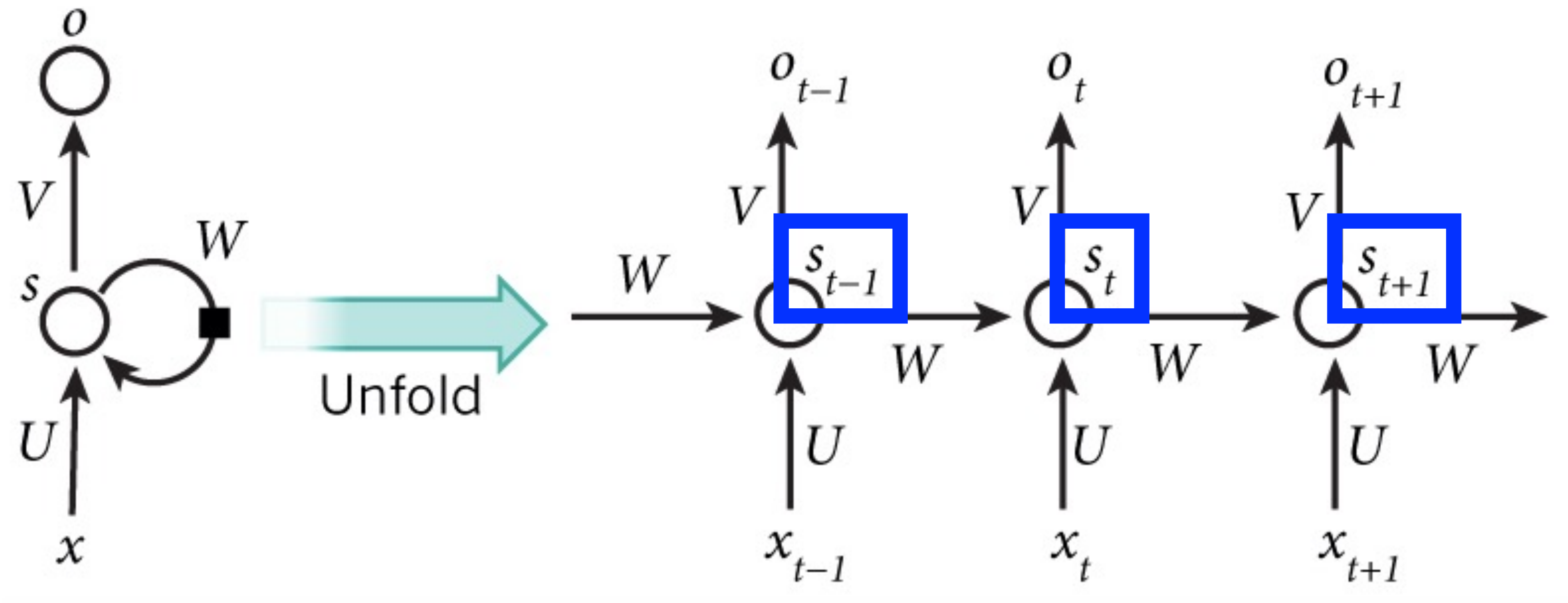
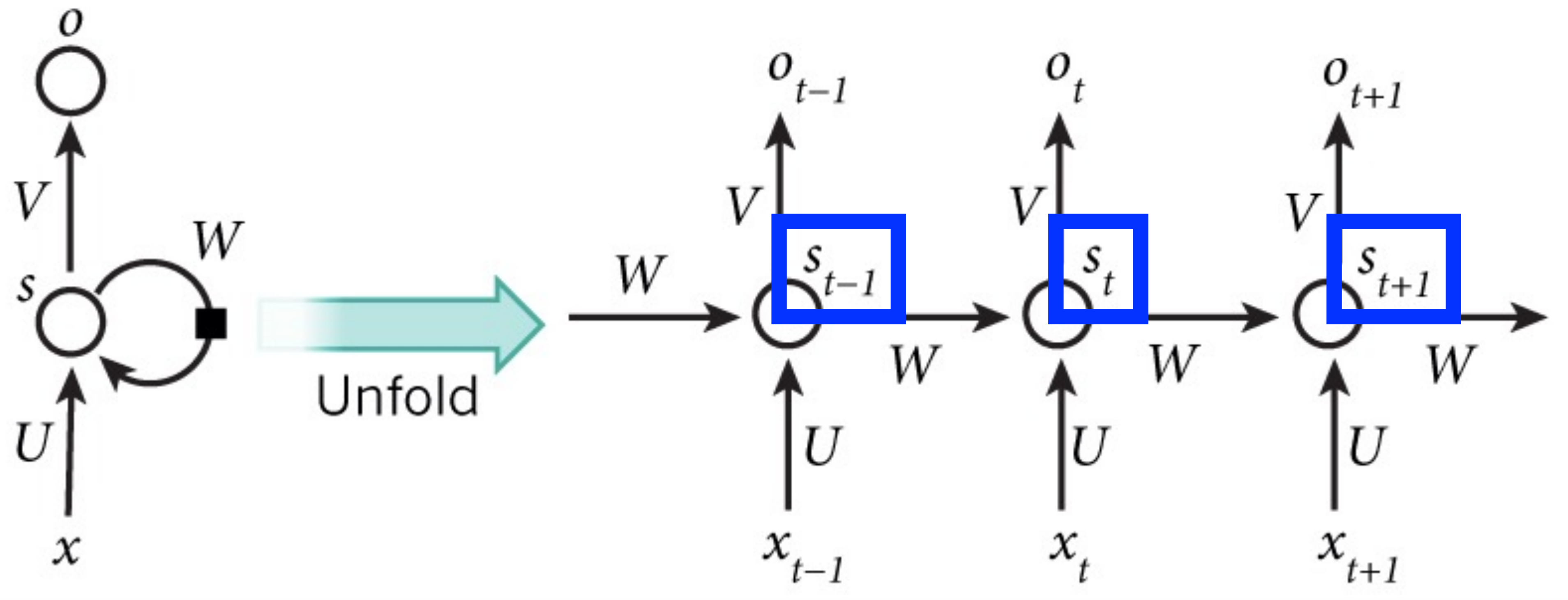
Goal: Model Sequential Data (Recall RNN)



Each hidden state is a function of the previous hidden state

http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-1-introduction-to-rnns/

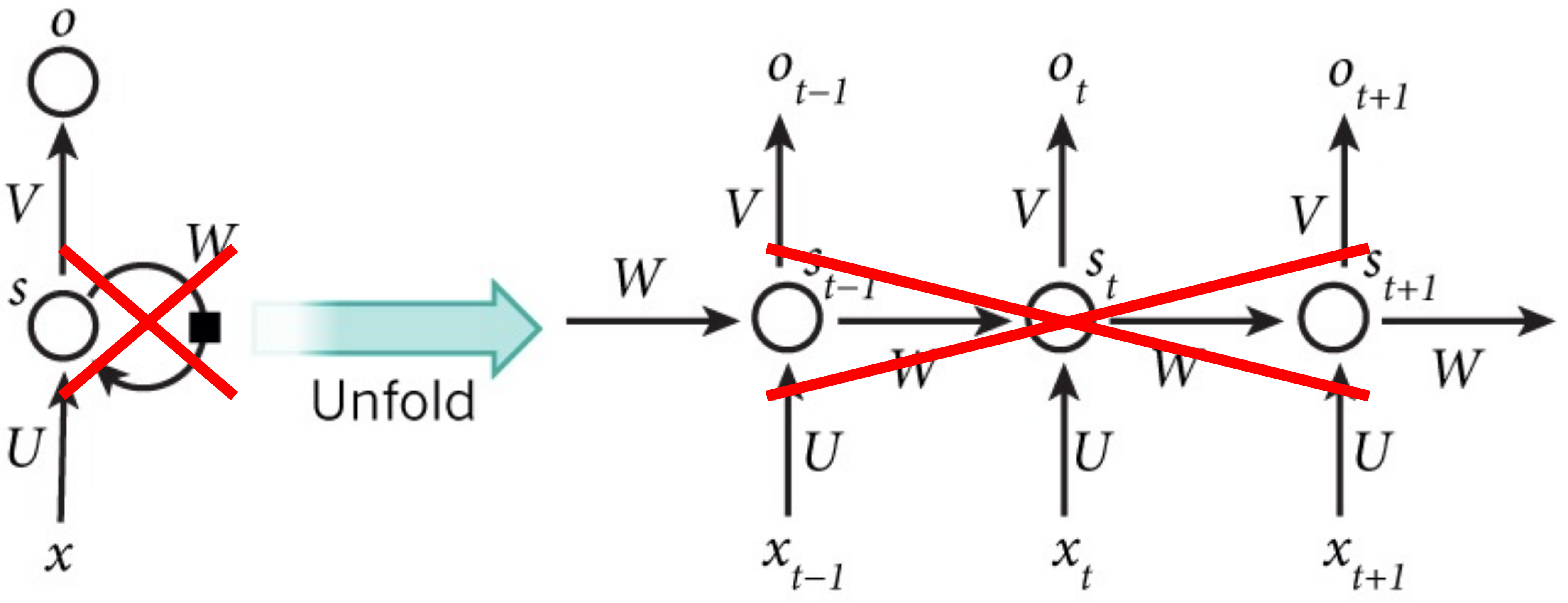
Problem: RNNs Use Sequential Computation



Seemingly hard for RNNs to carry information through hidden states across many time steps and train/testing is slow

http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-1-introduction-to-rnns/

Idea: Model Sequential Data Without Recurrence

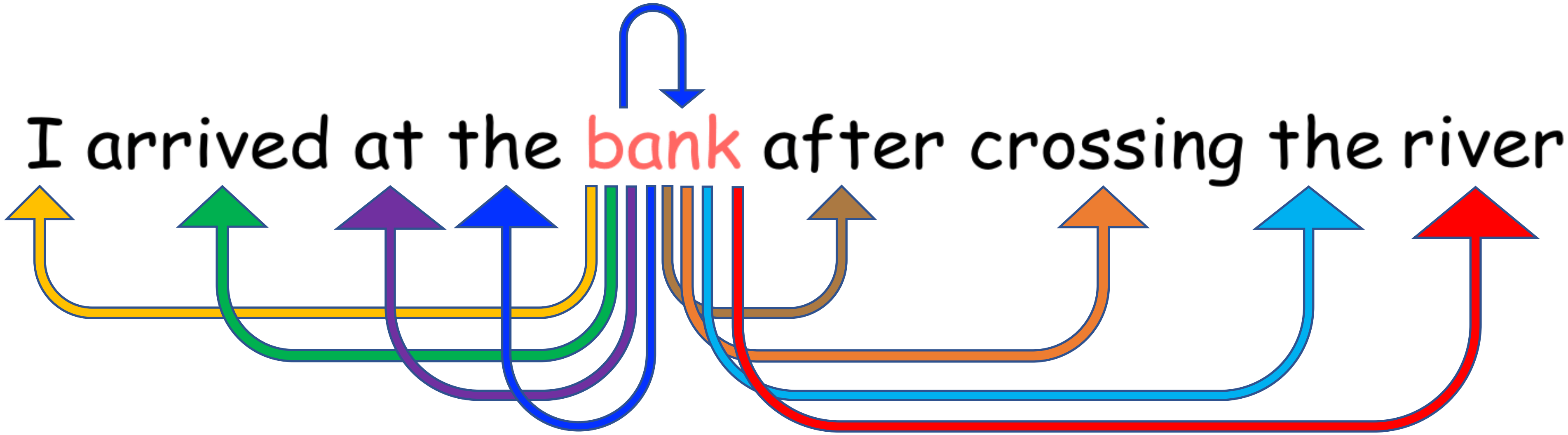


Replace sequential hidden states for capturing knowledge of other inputs with a new representation of each input that shows its relationship to all other inputs (i.e., self-attention)

http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-1-introduction-to-rnns/

Transformer Key Idea: Self-Attention

New representation of each token in a sequence showing its relationship to all tokens; e.g.,



https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

Transformer Key Idea: Self-Attention

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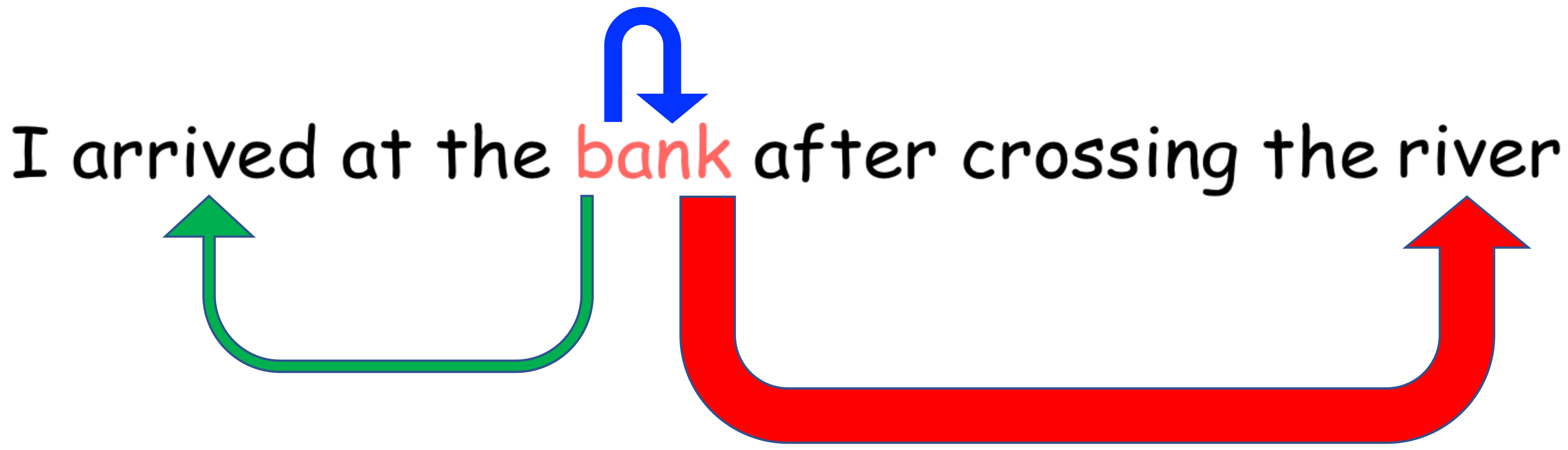

Arrow thickness is indicative of attention weight

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Transformer Key Idea: Self-Attention

New representation of each token in a sequence showing its relationship to all tokens; e.g.,

I arrived at the bank after crossing the river

A large attention score means the other word will strongly inform the new representation of the word

https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

Transformer Intuition

What does bank mean in this sentence?

I arrived at the bank after crossing the …

https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

Transformer Intuition

What does bank mean in this sentence?
- new word representation disambiguates meaning by identifying other relevant words (e.g., high attention score with “river”)

I arrived at the bank after crossing the river

vs

I arrived at the bank after crossing the street

https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

Transformer vs RNN (Intuition)

I arrived at the bank after crossing the …

$\boxed{\text{...street?} \quad \text{...river?}}$

What does **bank** mean in this sentence? Meaning depends on other input words

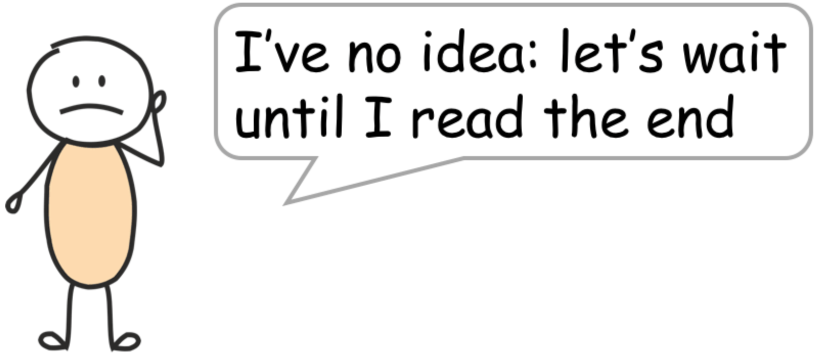
https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

Transformer vs RNN (Intuition)

I arrived at the bank after crossing the …

…street? …river?

What does **bank** mean in this sentence? Meaning depends on other input words



RNNs

O(N) steps to process a sentence with length N

Transformer

Constant number of steps to process any sentence

https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

Transformer: A Suggested Definition

"Any architecture designed to process a connected set of units—such as the tokens in a sequence or the pixels in an image—where the only interaction between units is through self-attention."

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- Common transformer ingredients
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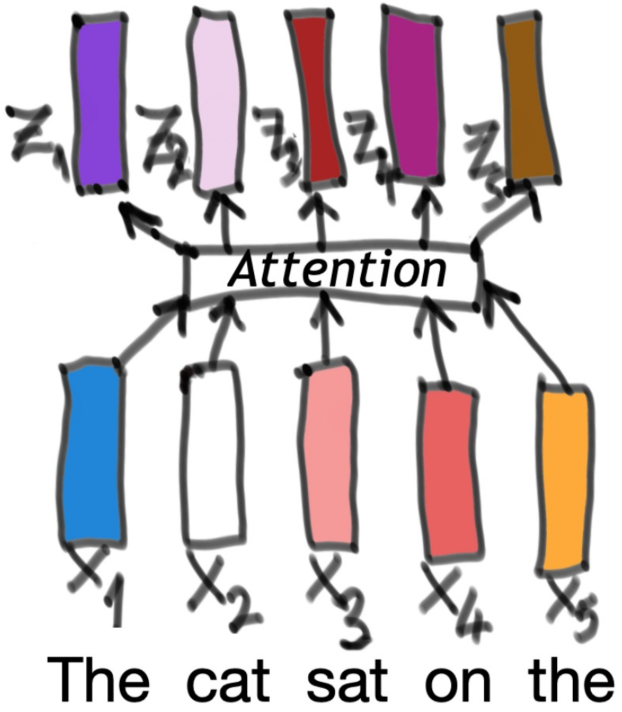
Self-Attention: Outcome

New representation of each token in a sequence showing its relationship to all tokens



https://towardsdatascience.com/self-attention-5b95ea164f61

Self-Attention: Outcome

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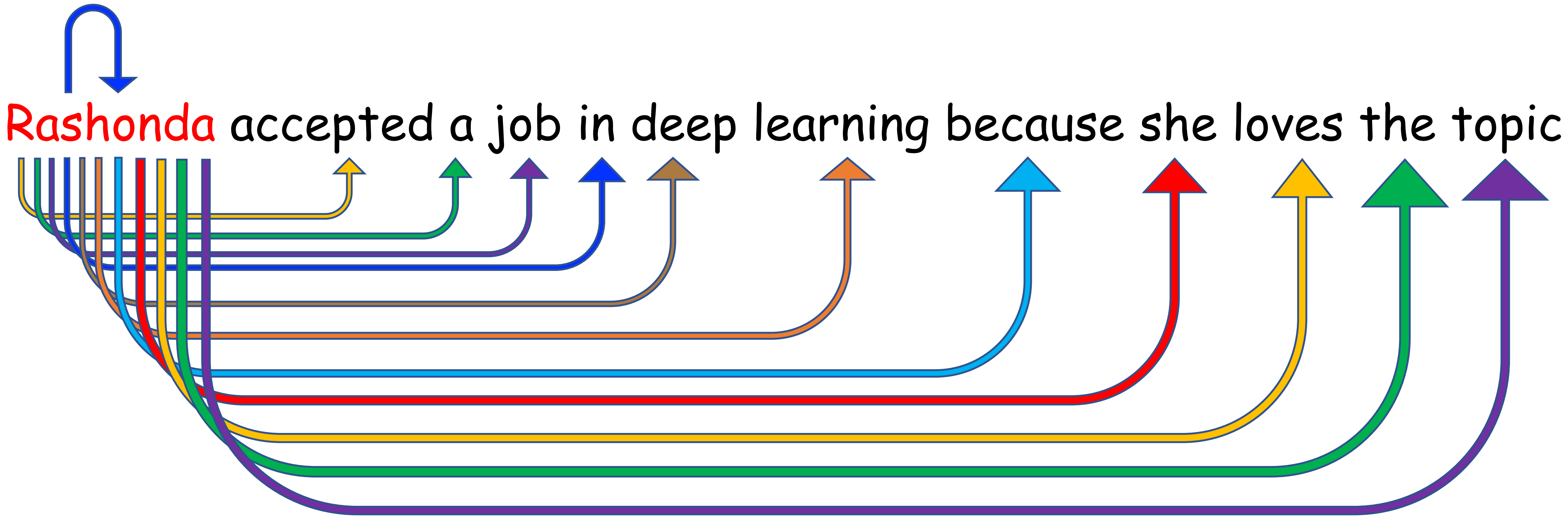

Self-Attention: Outcome

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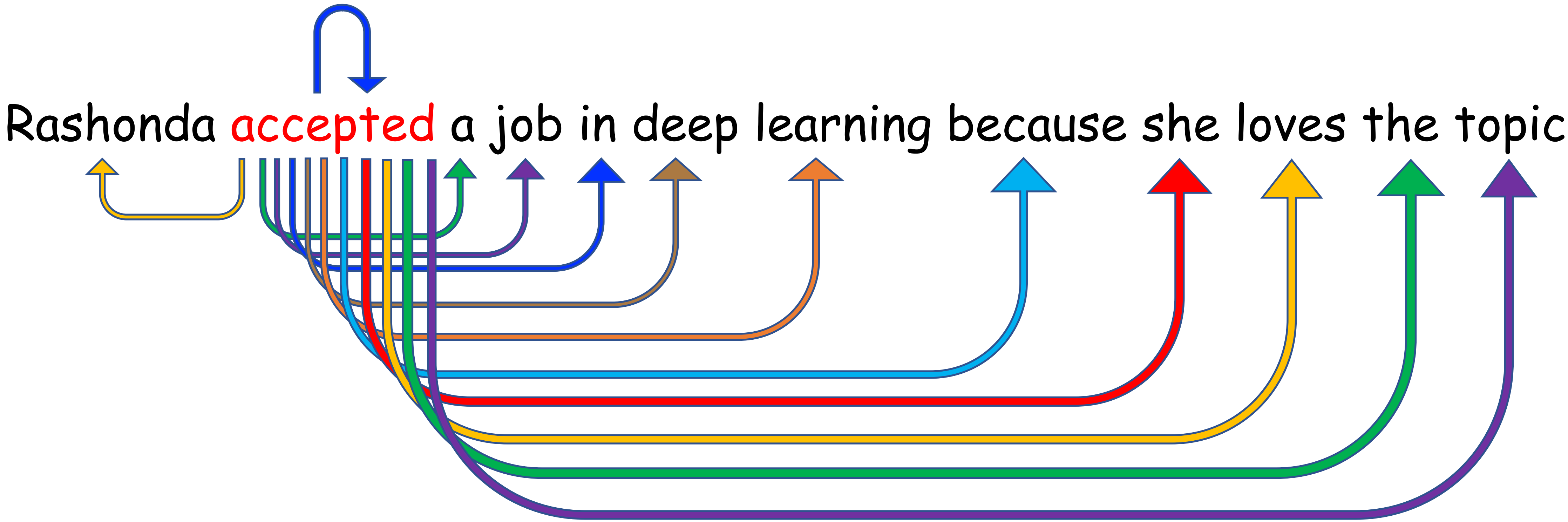


Self-Attention: Outcome

New representation of each token in a sequence showing its relationship to all tokens; e.g.,

Rashonda accepted a job in deep learning because she loves the topic

And so on for remaining words…

Self-Attention: Disambiguates Word Meanings

New representation of each token in a sequence showing its relationship to all tokens; e.g.,

Rashonda accepted a job in deep learning because she loves the topic

A better representation of "she" would encode information about "Rashonda"

Self-Attention: Disambiguates Word Meanings

New representation of each token in a sequence showing its relationship to all tokens; e.g.,

I arrived at the bank across the river

Recall: a better representation of "bank" would encode information about "river"

https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html#transformer_intro

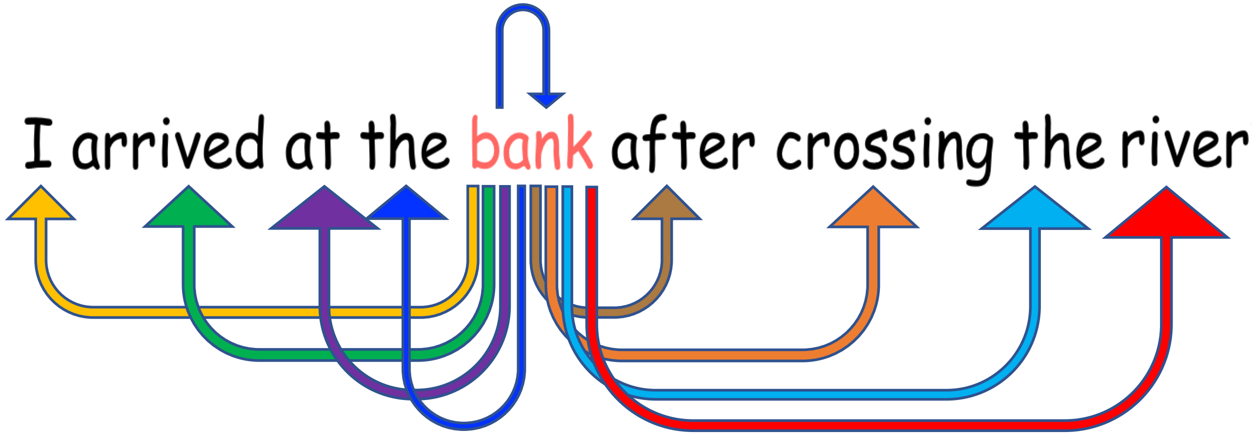
Self-Attention vs General Attention

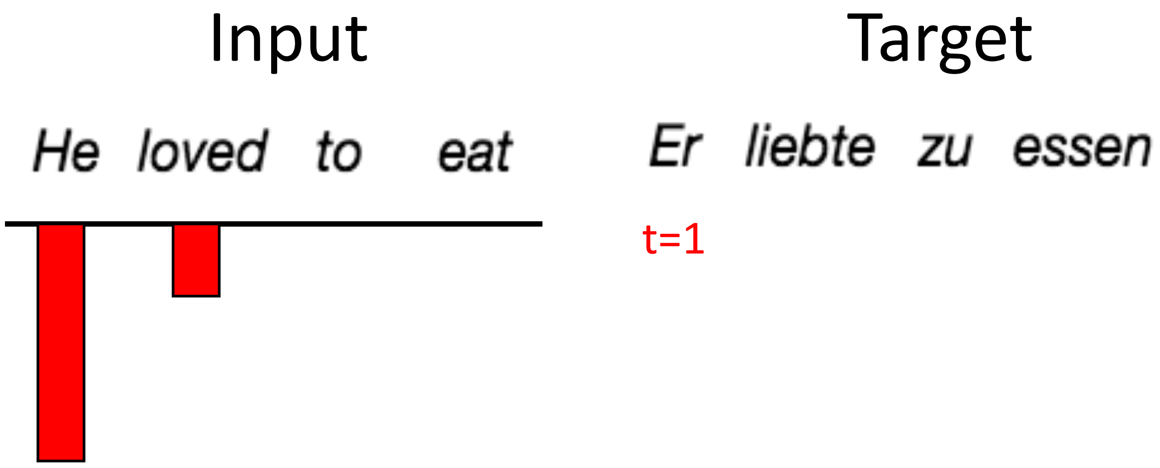
Self-attention

Relates tokens from the same source

General attention

Relates tokens from different sources





Computing Self-Attention: Similar Approach to How We Compute General Attention

Attention output

$$\boxed{c^{(t)} = a_1^{(t)} s_1 + a_2^{(t)} s_2 + \cdots + a_m^{(t)} s_m = \sum_{k=1}^{m} a_k^{(t)} s_k}$$

"source context for decoder step t"

(weighted sum)

Key difference 2: attention score multiplied with a value derived from the input

Attention weights

$$a_k^{(t)} = \frac{\exp(\mathrm{score}(h_t, s_k))}{\sum_{i=1}^{m} \exp(\mathrm{score}(h_t, s_i))}, \mathrm{k} = 1..\mathrm{m}$$

"attention weight for source token k at decoder step t"

(softmax)

Attention scores

$\mathrm{score}(h_t, s_k), \mathrm{k} = 1..\mathrm{m}$

"How relevant is source token k for target step t?"

Attention input

$s_1, s_2, \ldots, s_m$ — all encoder states

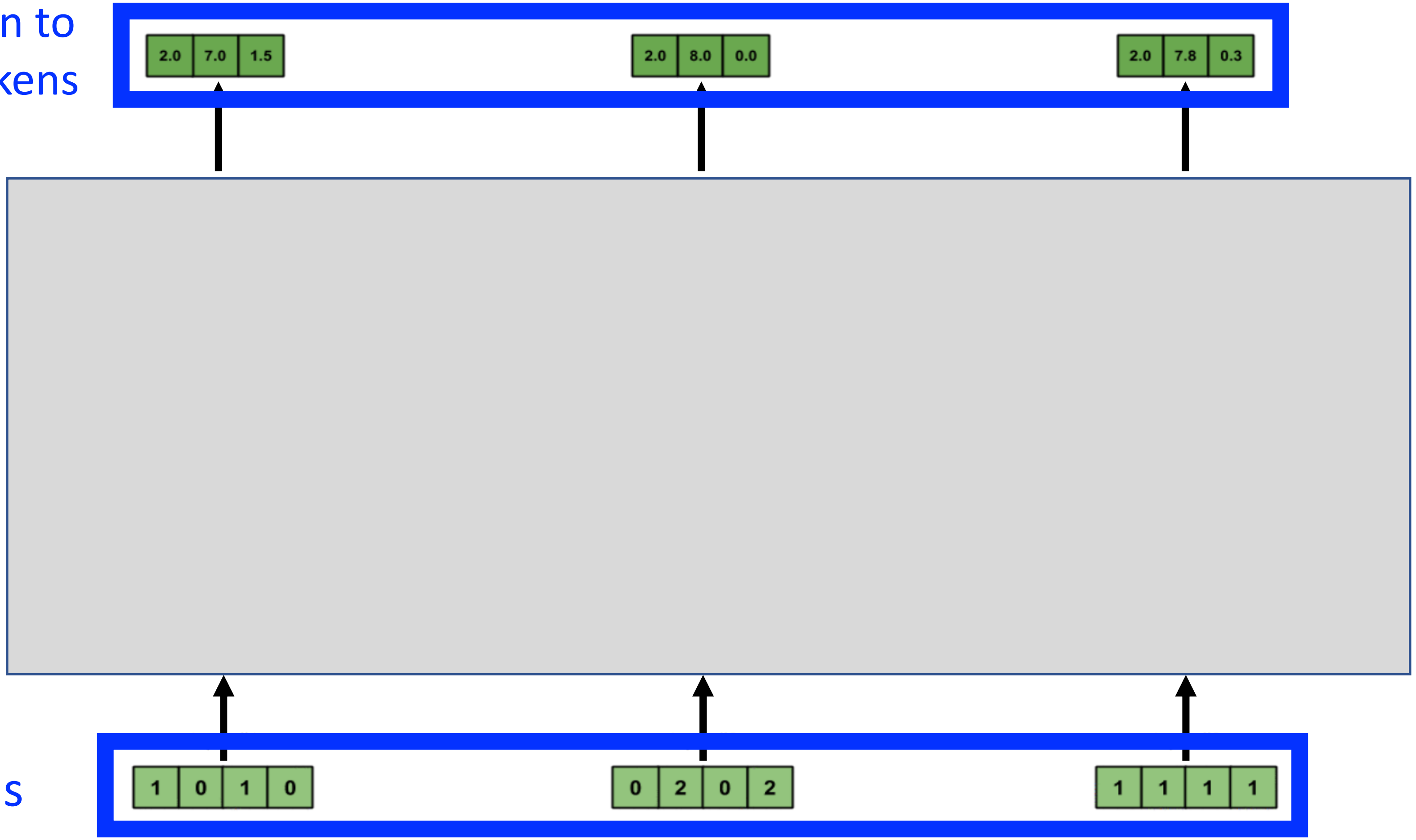
h_t — one decoder state

Key difference 1: input for self-attention

https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html

Computing Self-Attention: Example

New representation of each input token to reflect each one's relationship to all tokens



Input tokens

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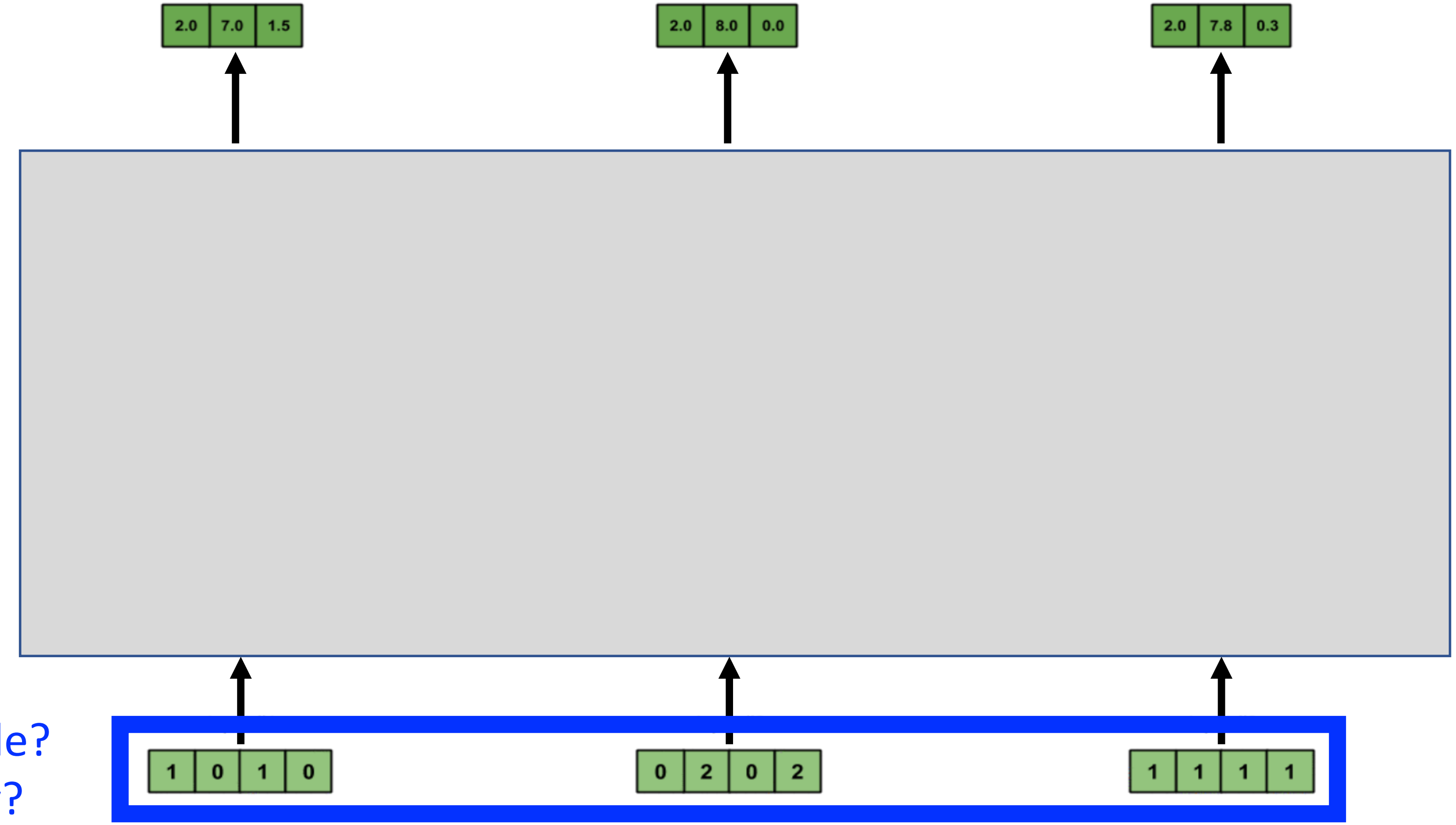
Computing Self-Attention: Example



- How many inputs are in this example?
- What is each input's dimensionality?

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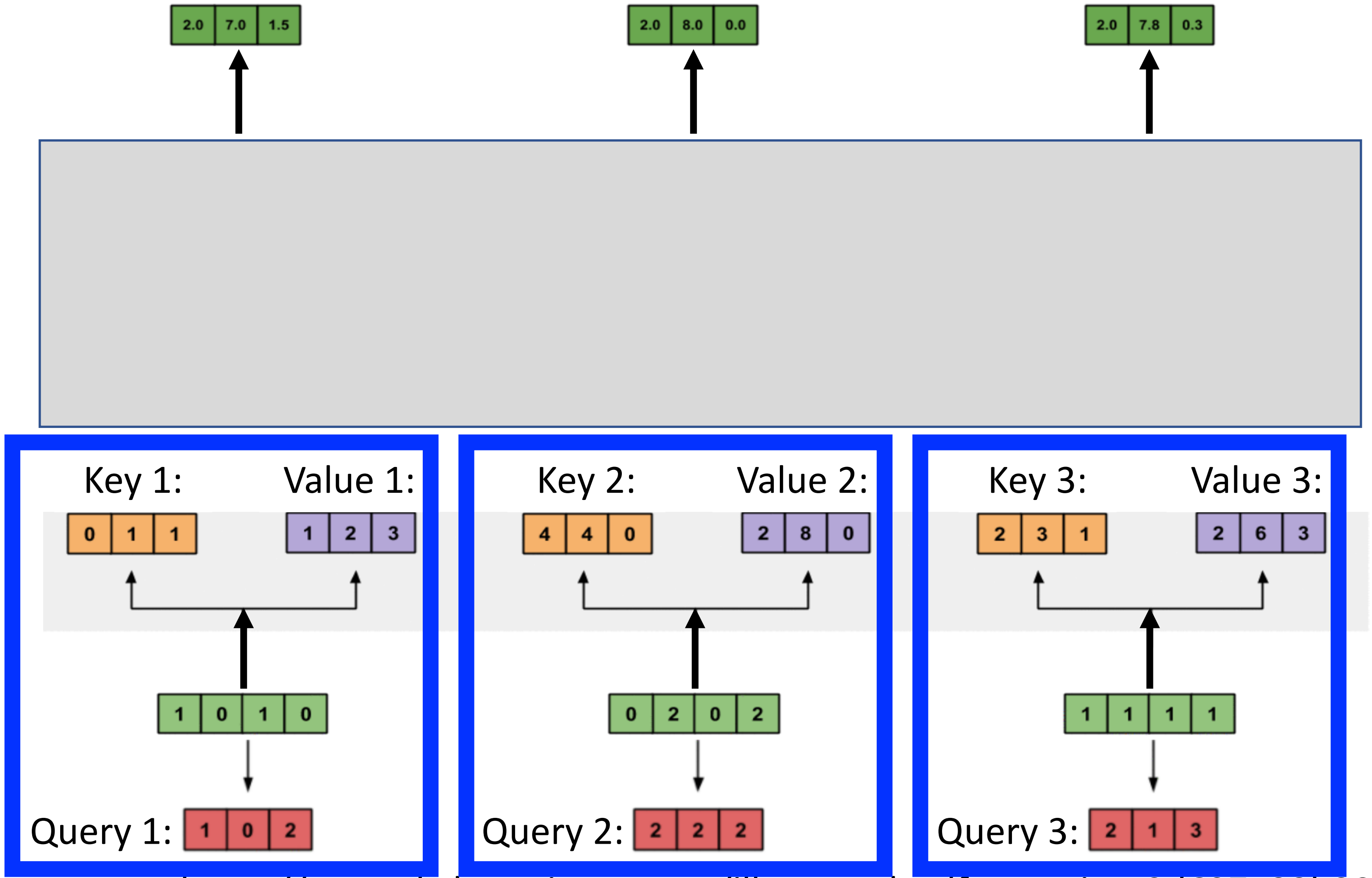
Computing Self-Attention: Example



Three vectors are derived for each input by multiplying with three weight matrices (learned during training): query, key, and value

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Computing Self-Attention: Example

e.g., key weights

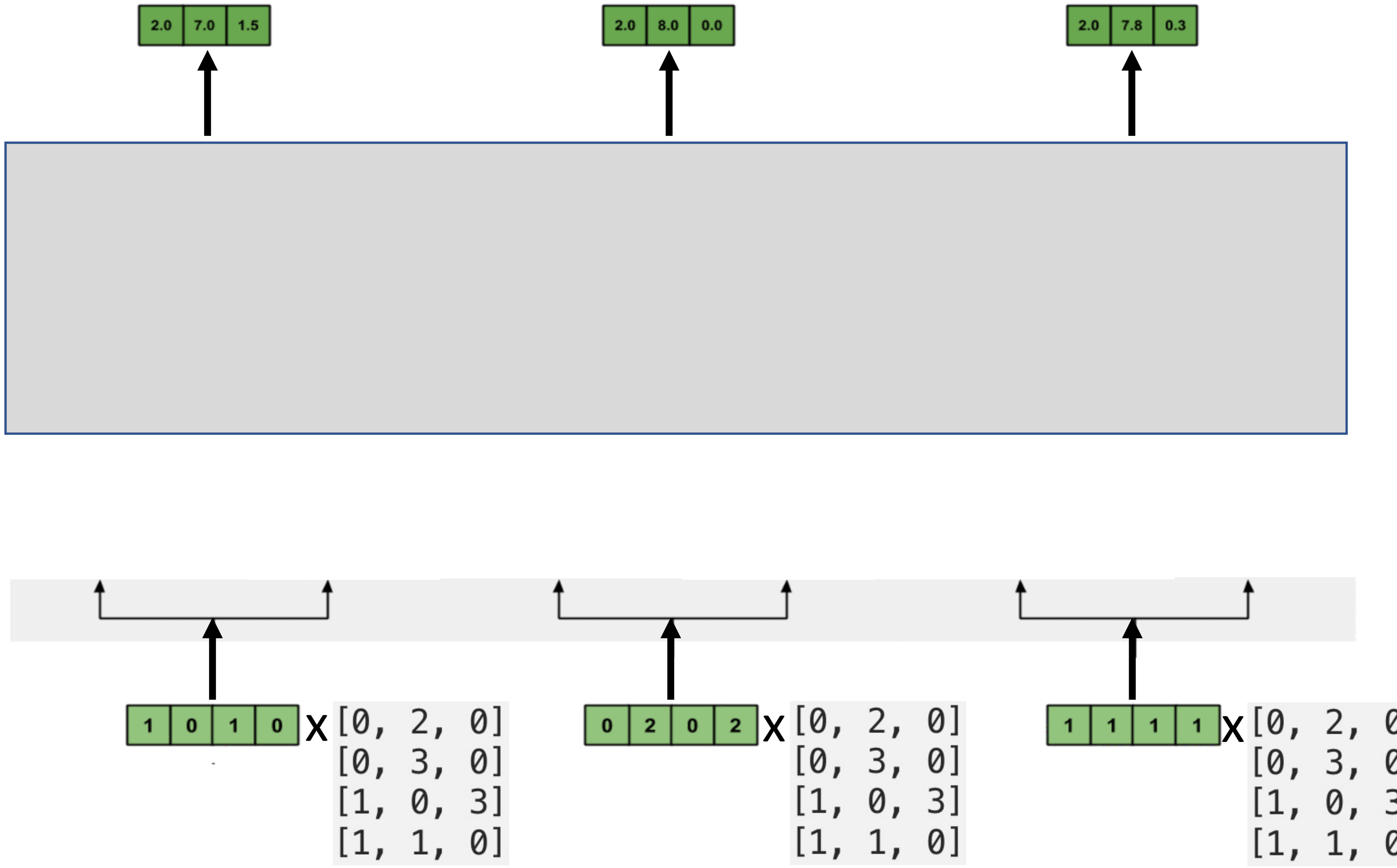
```
[0, 0, 1]
[1, 1, 0]
[0, 1, 0]
[1, 1, 0]
```

https://towardsdatascience.com/illustrated-self-attention-2d627e33b20a

Computing Self-Attention: Example

e.g., value weights

```
[0, 2, 0]
[0, 3, 0]
[1, 0, 3]
[1, 1, 0]
```



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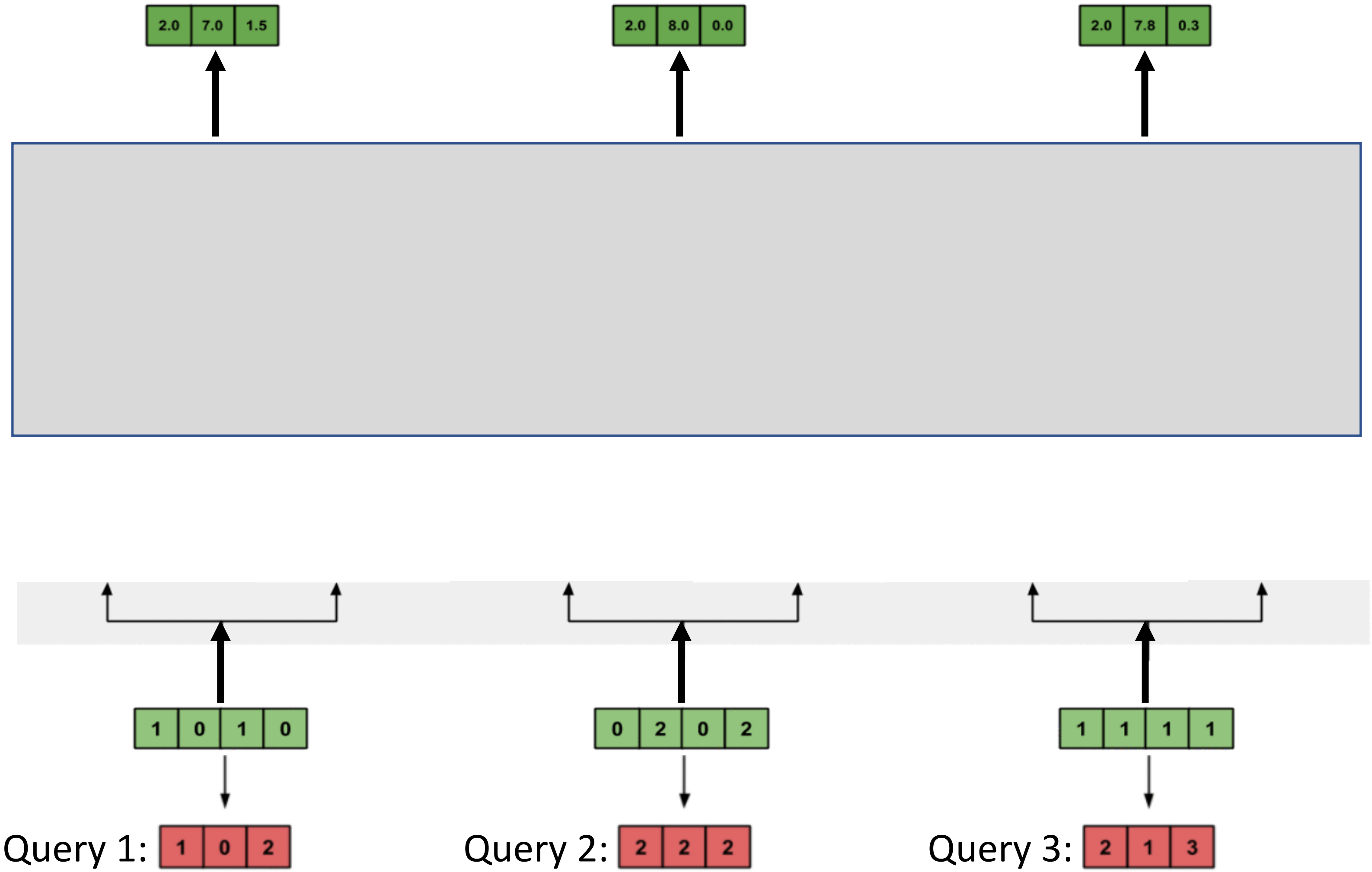
Computing Self-Attention: Example

e.g., query weights

```
[1, 0, 1]
[1, 0, 0]
[0, 0, 1]
[0, 1, 1]
```



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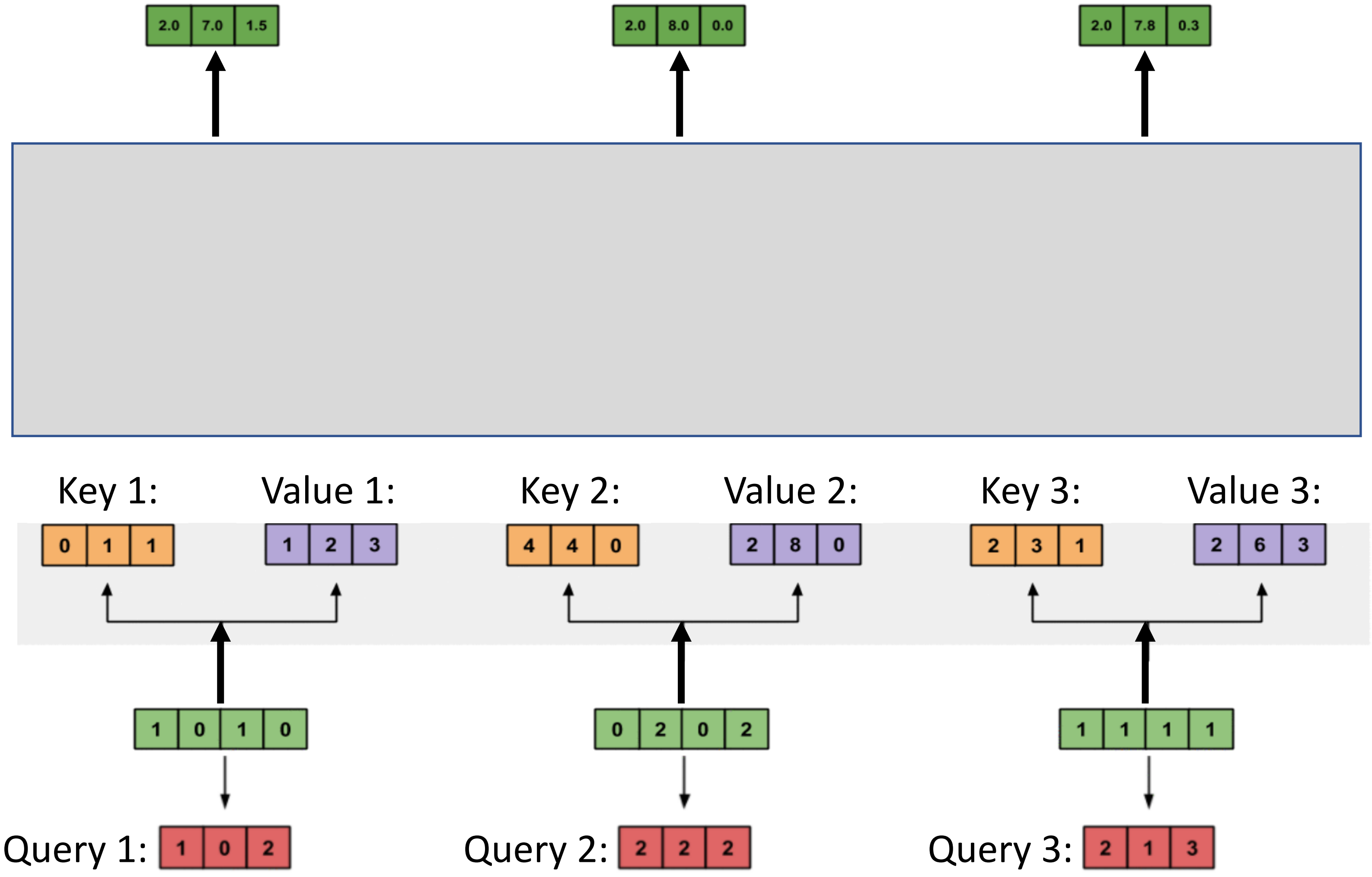
Computing Self-Attention: Example



How many weight matrices are learned in this example?

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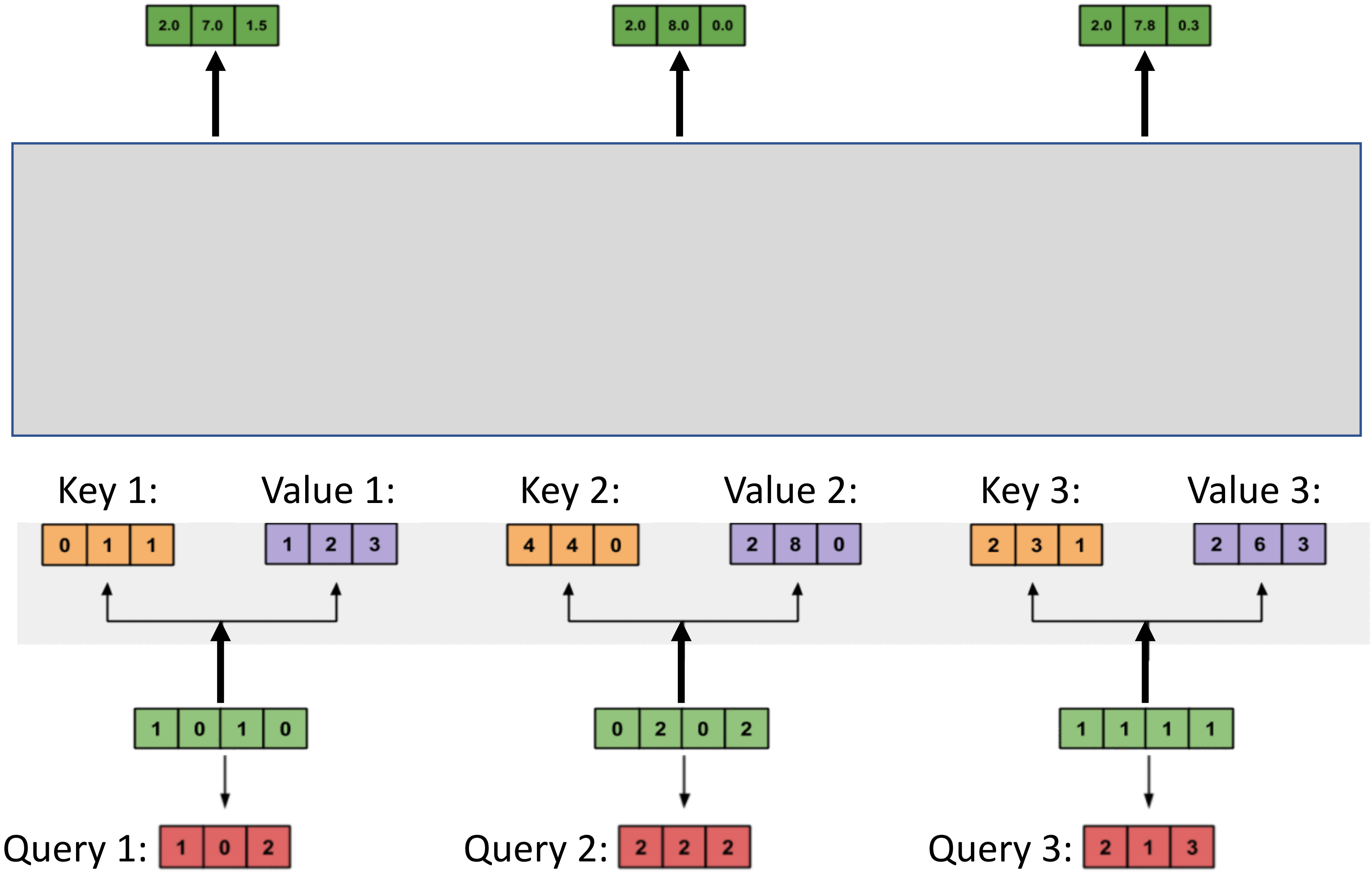
Computing Self-Attention: Example

What is the purpose of the three weight matrices?

For each input, 2 of the derived vectors are used to compute **attention weights** (query and key) and the 3rd is **information** passed on for the new representation (value)



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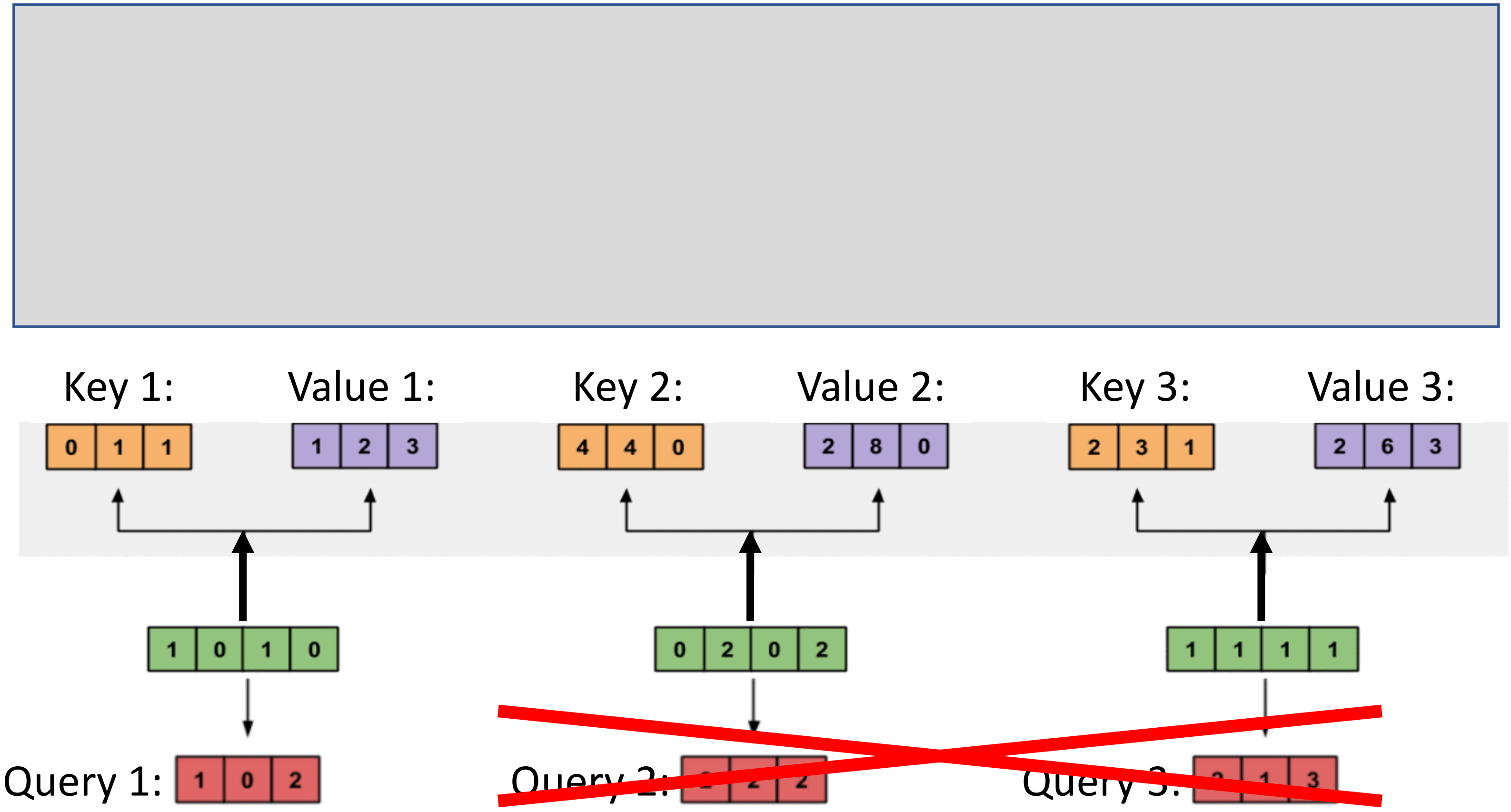
Computing Self-Attention: Example



We now will examine how to find the new representation for the first input.

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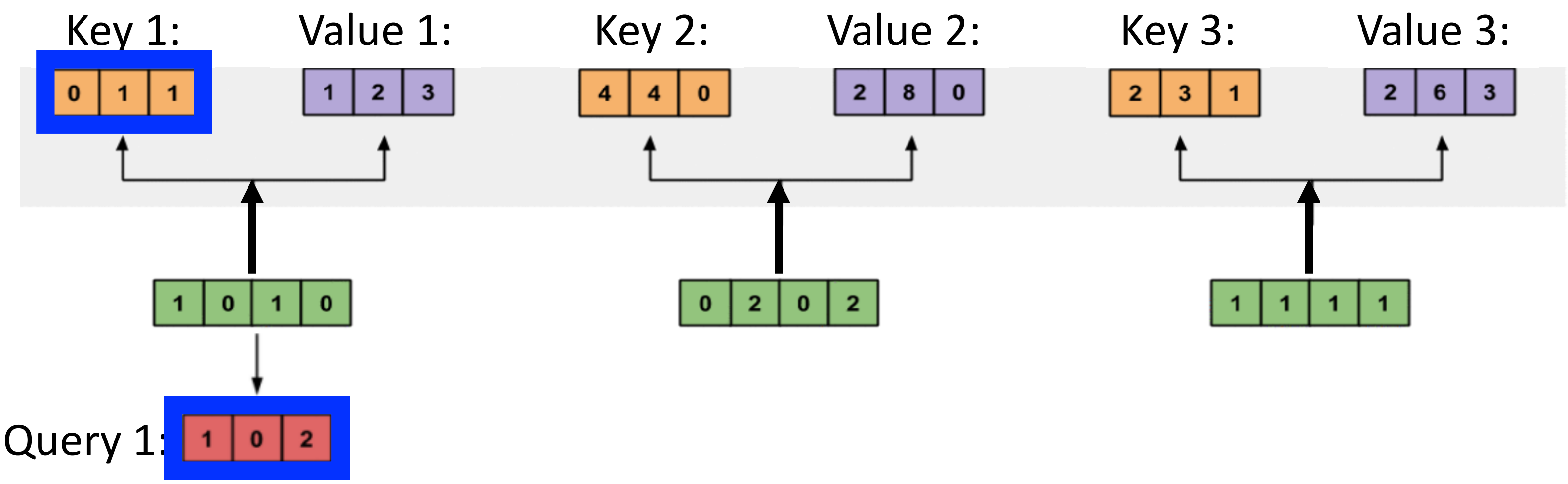
Computing Self-Attention: Example

Attention score: dot product of query with all keys to identify relevant tokens; e.g.,

$$\begin{bmatrix}1 & 0 & 2\end{bmatrix} \times \begin{bmatrix}0\\1\\1\end{bmatrix} = ?$$



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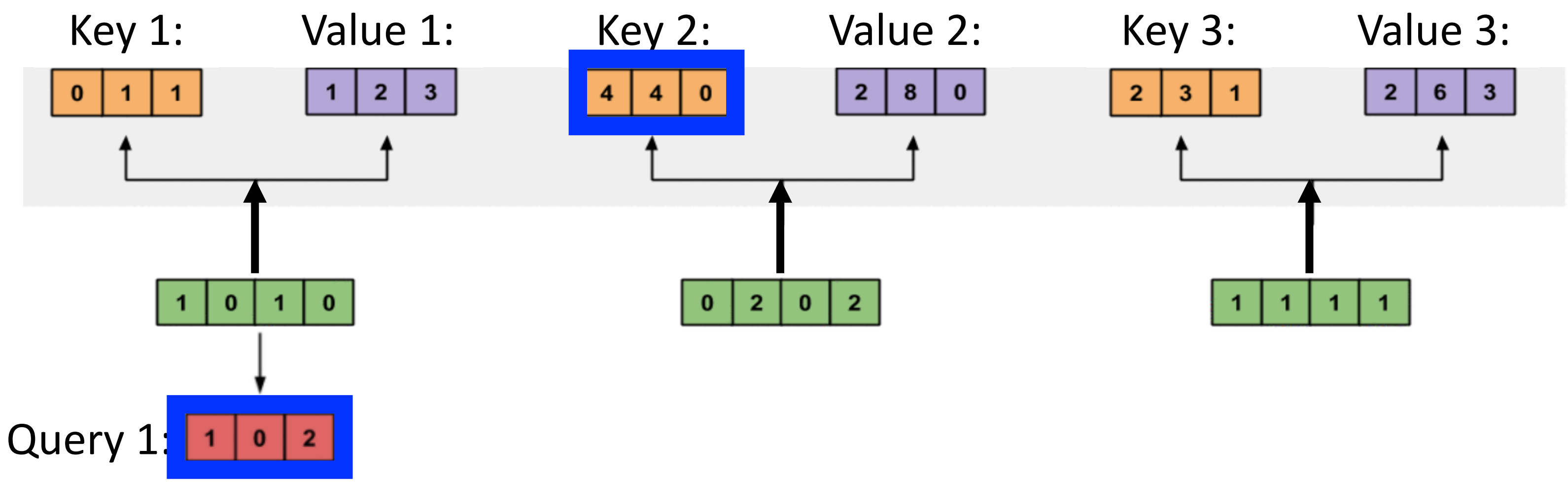
Computing Self-Attention: Example

Attention score: dot product of query with all keys to identify relevant tokens; e.g.,

$$\begin{bmatrix} 1 & 0 & 2 \end{bmatrix} \times \begin{bmatrix} 4 \\ 4 \\ 0 \end{bmatrix} = ?$$



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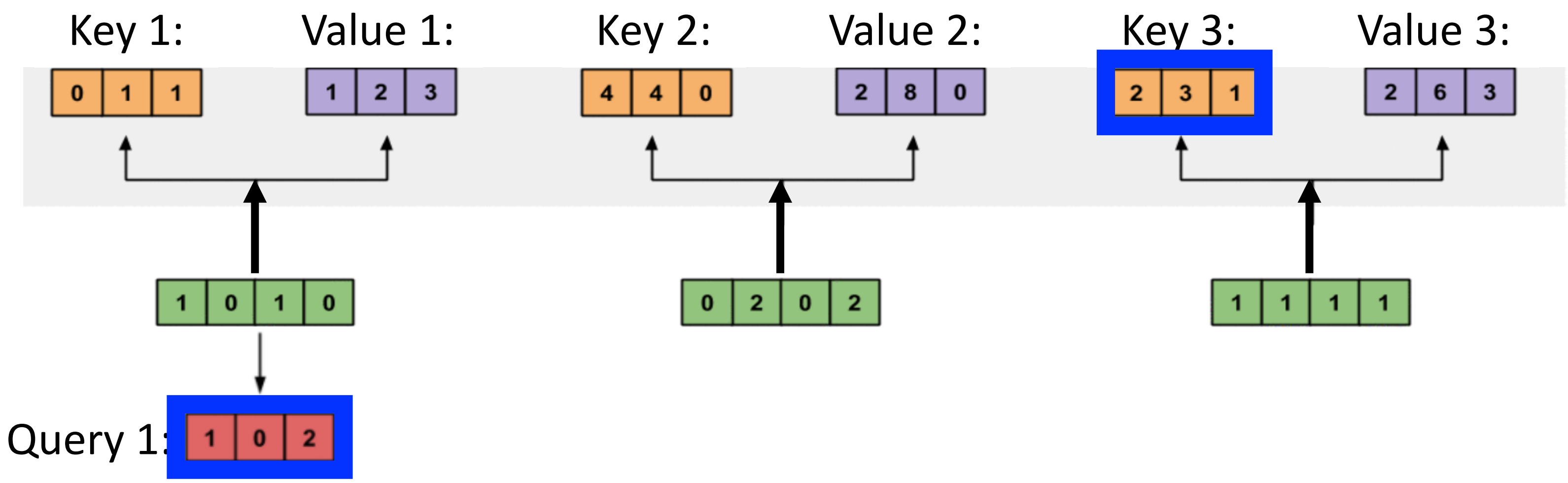
Computing Self-Attention: Example

Attention score: dot product of query with all keys to identify relevant tokens; e.g.,

$$\begin{bmatrix} 1 & 0 & 2 \end{bmatrix} \times \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix} = ?$$



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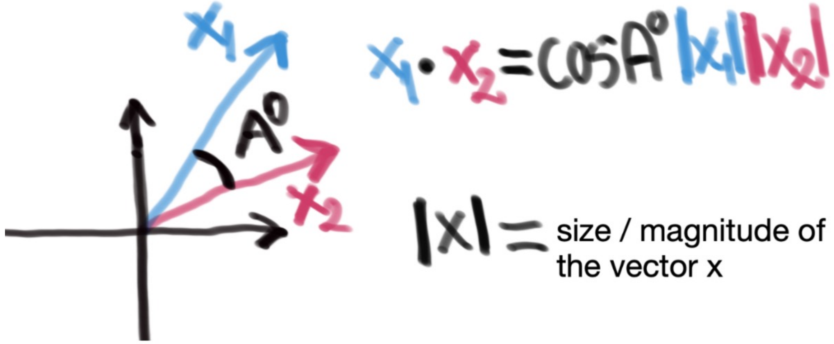
Computing Self-Attention: Example

Why dot product? Indicates similarity of two vectors

- Match = 1 (i.e., cos(0))
- Opposites = -1 (i.e., cos(180))



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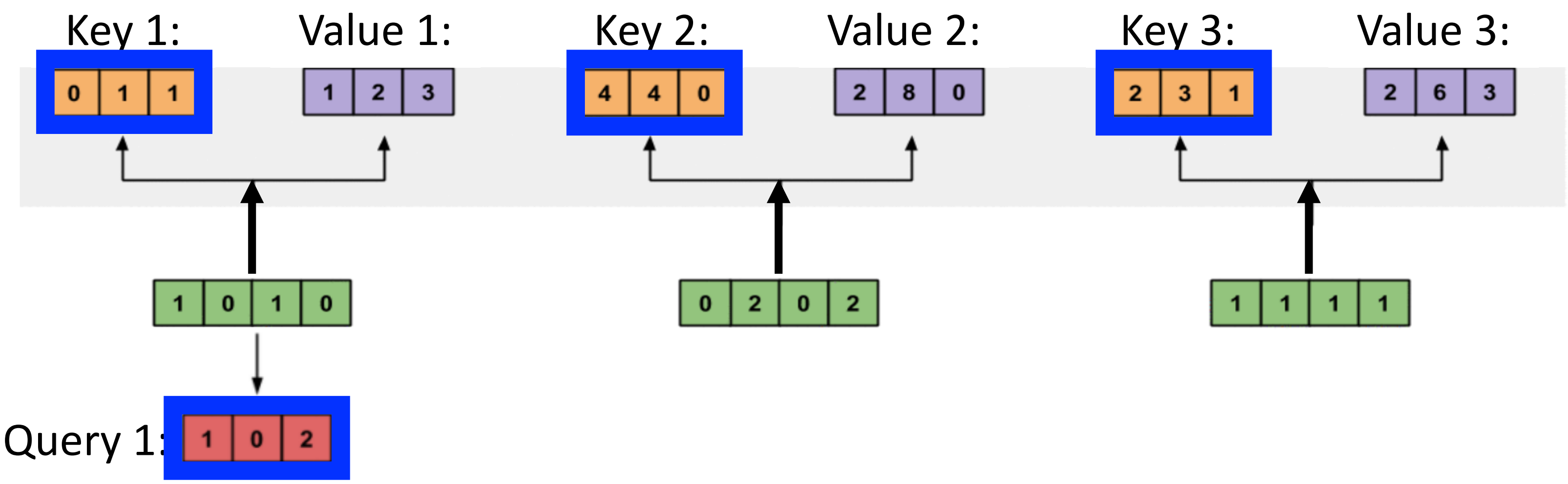

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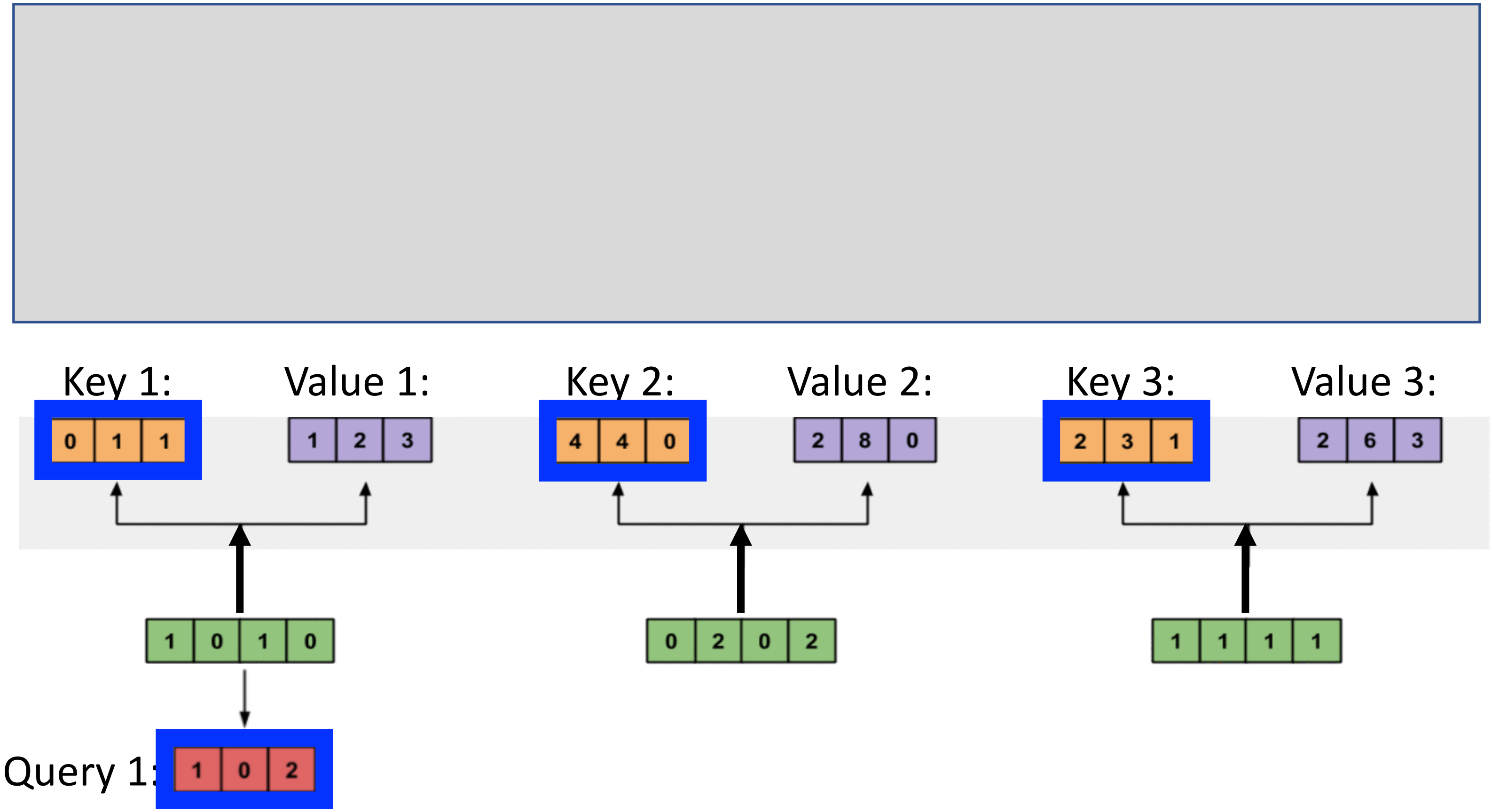
Computing Self-Attention: Example

Can use similarity measures other than the dot product



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Computing Self-Attention: Example

Attention weights: softmax scores for all inputs to quantify each token's relevance; e.g.,

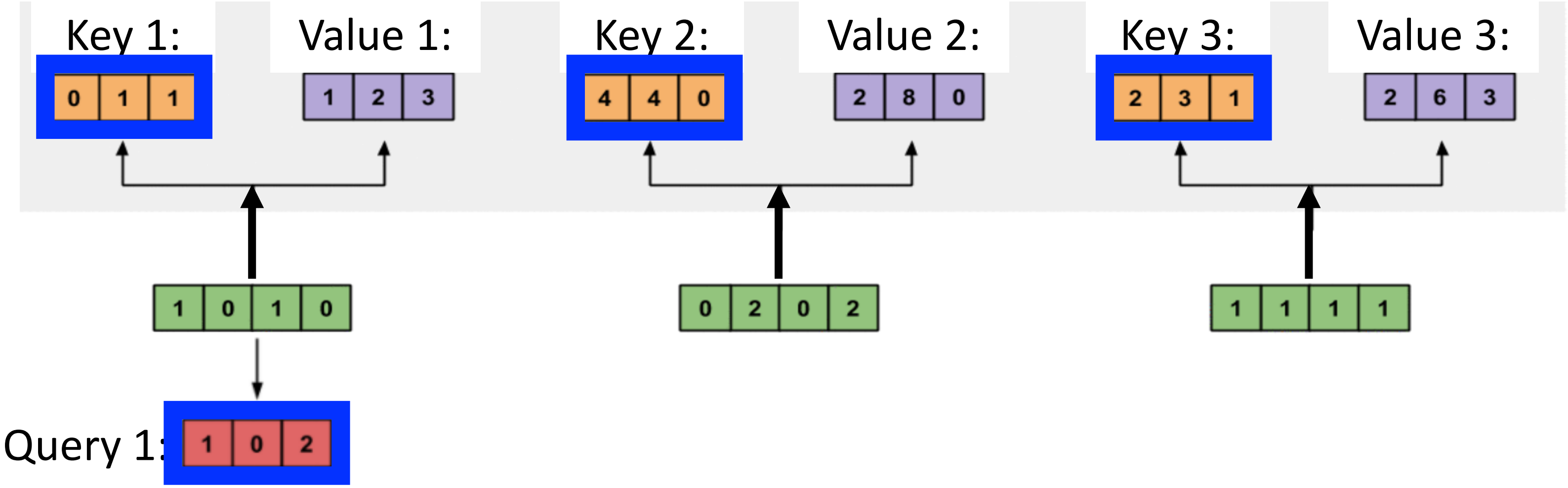
= softmax([2, 4, 4])

= $\boxed{\text{[0.0, 0.5, 0.5]})}$

Note: softmax doesn't return 0, but can arise from rounding

To which input(s) is input 1 **least** related?

To which input(s) is input 1 **most** related?



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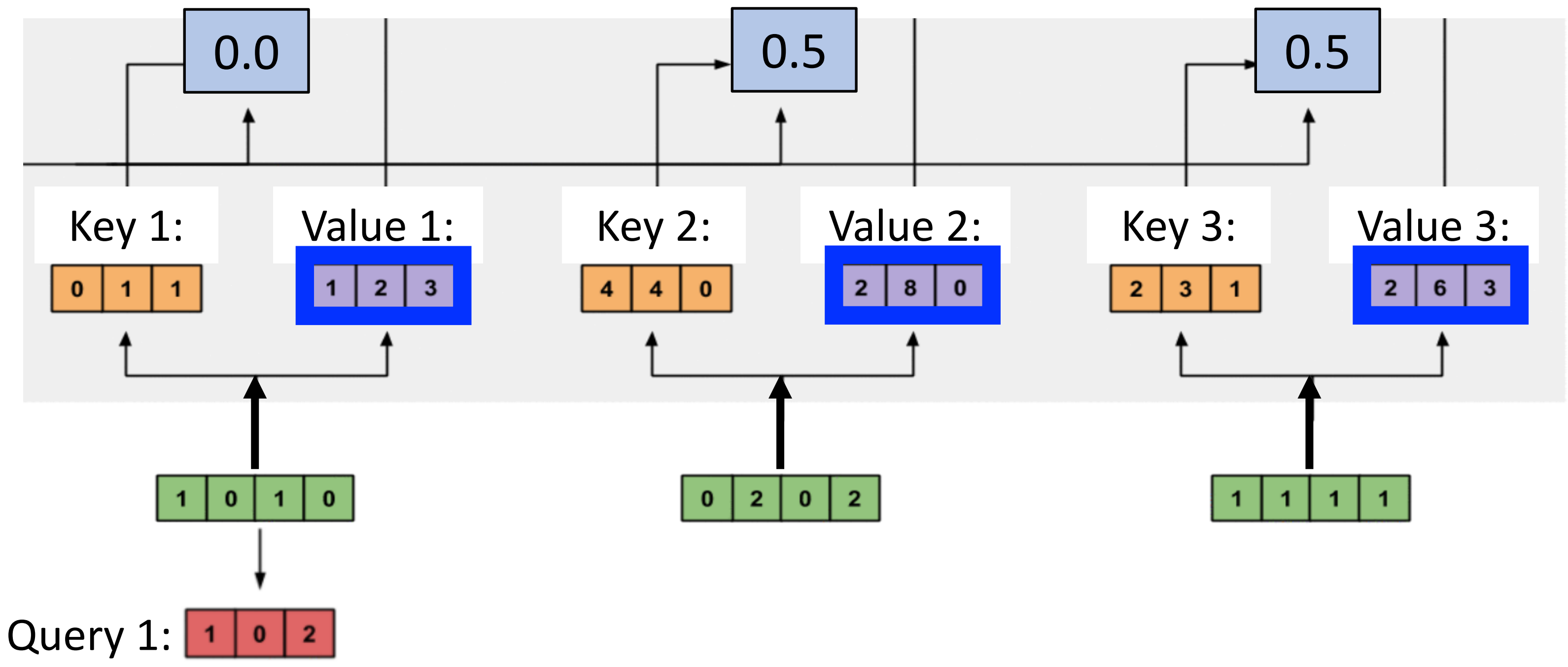
Computing Self-Attention: Example

Compute new representation of input token that reflects entire input:

1. Attention weights x Values



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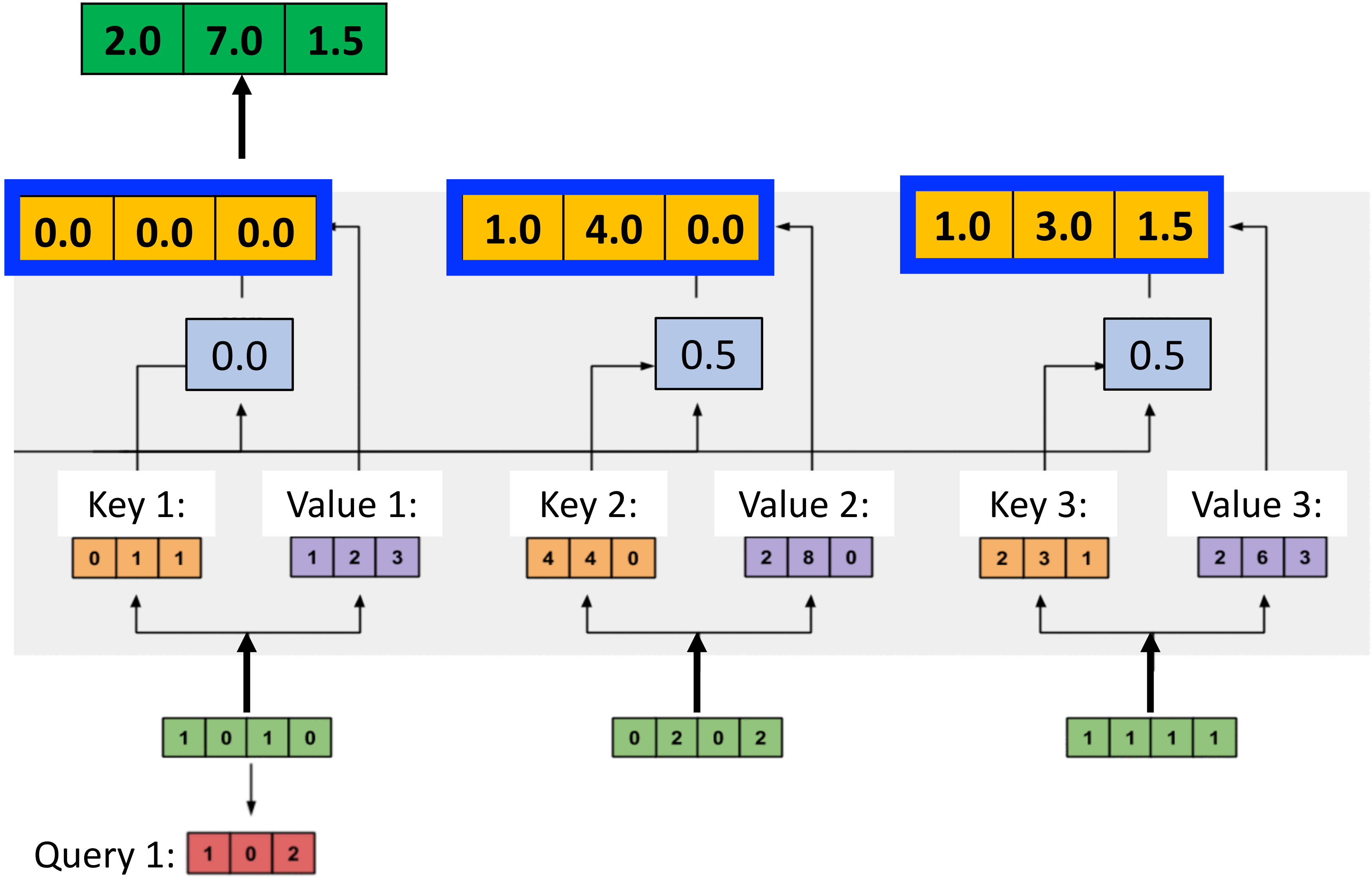
Computing Self-Attention: Example

Compute new representation of input token that reflects entire input:

1. Attention weights x Values

2. Sum all weighted vectors



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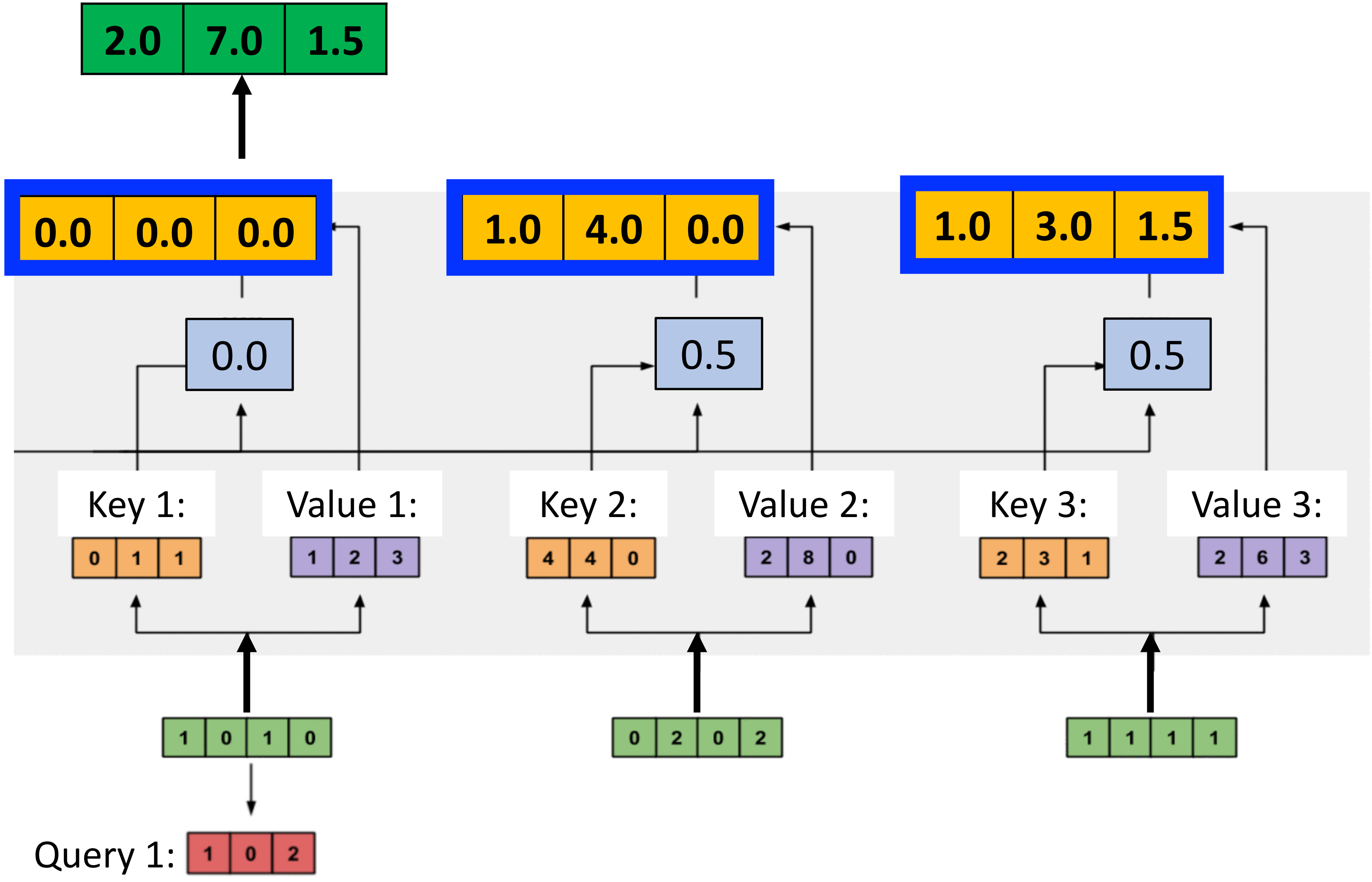
Computing Self-Attention: Example

Attention weights amplify input representations (values) that we want to pay attention to and repress the rest



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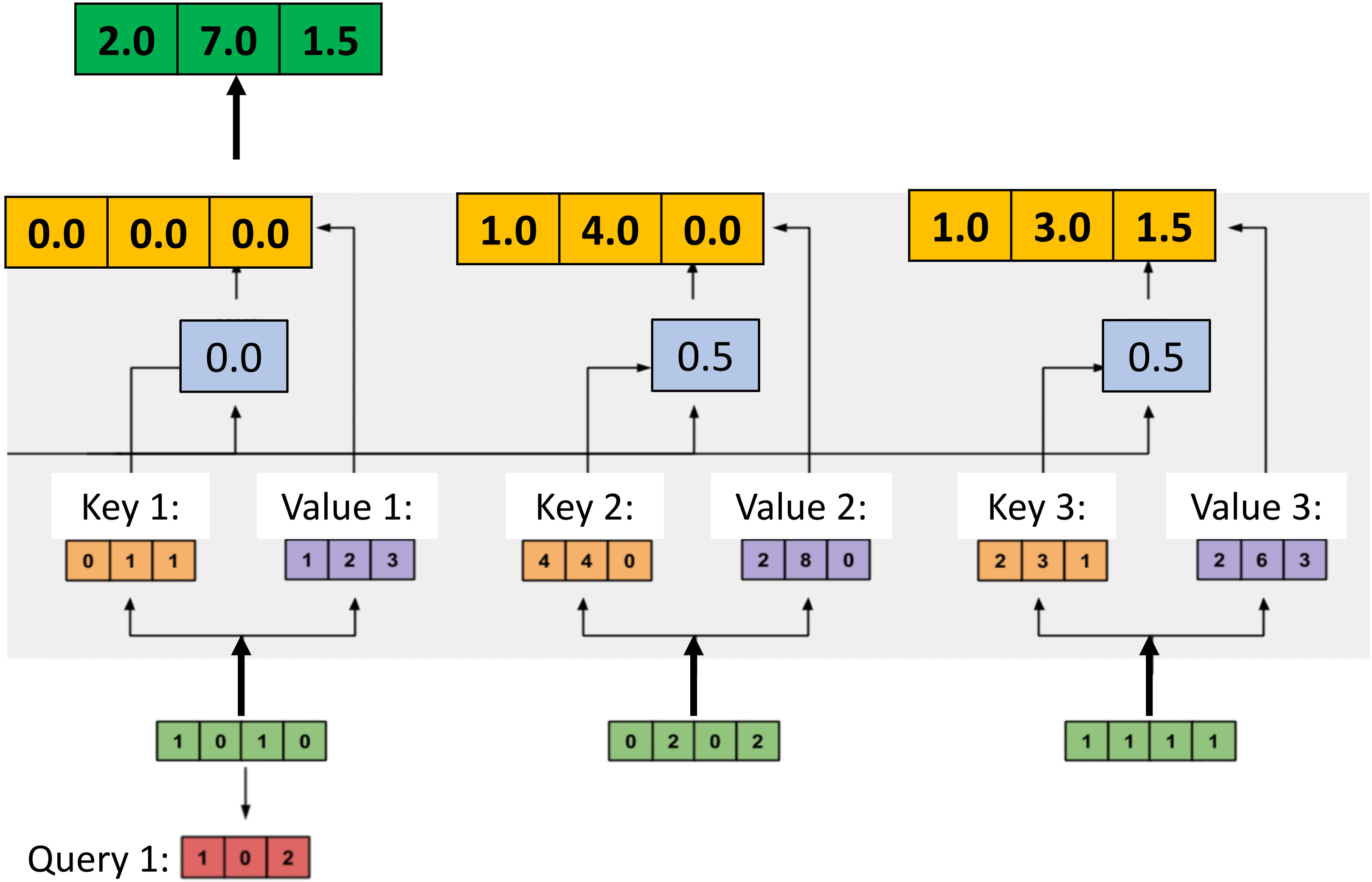

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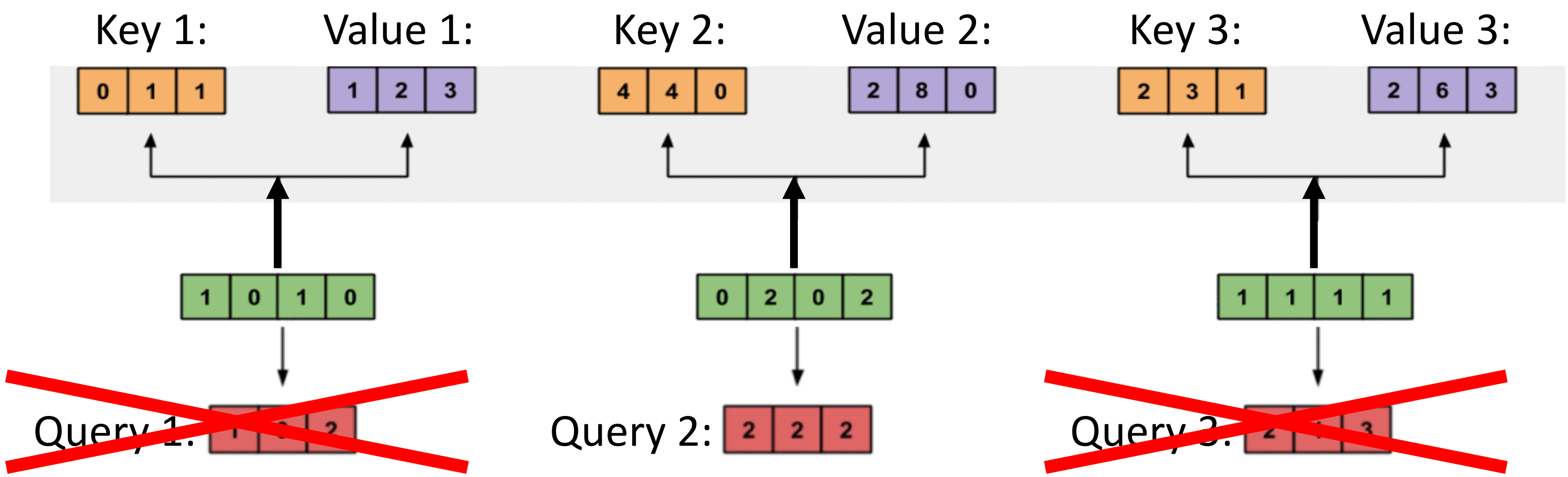
Computing Self-Attention: Example

Repeat the same process for each remaining input token



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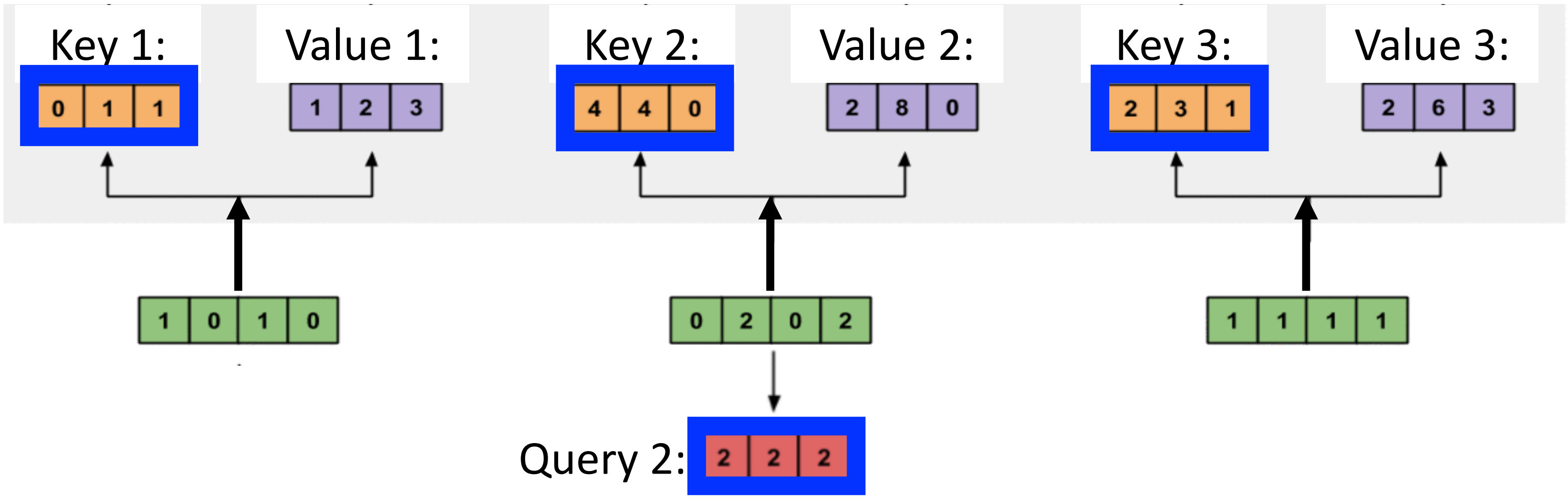
Computing Self-Attention: Example

1. Compute attention weights
- Softmax resulting 3 scores from query x keys

To which input(s) is input 2 most related?



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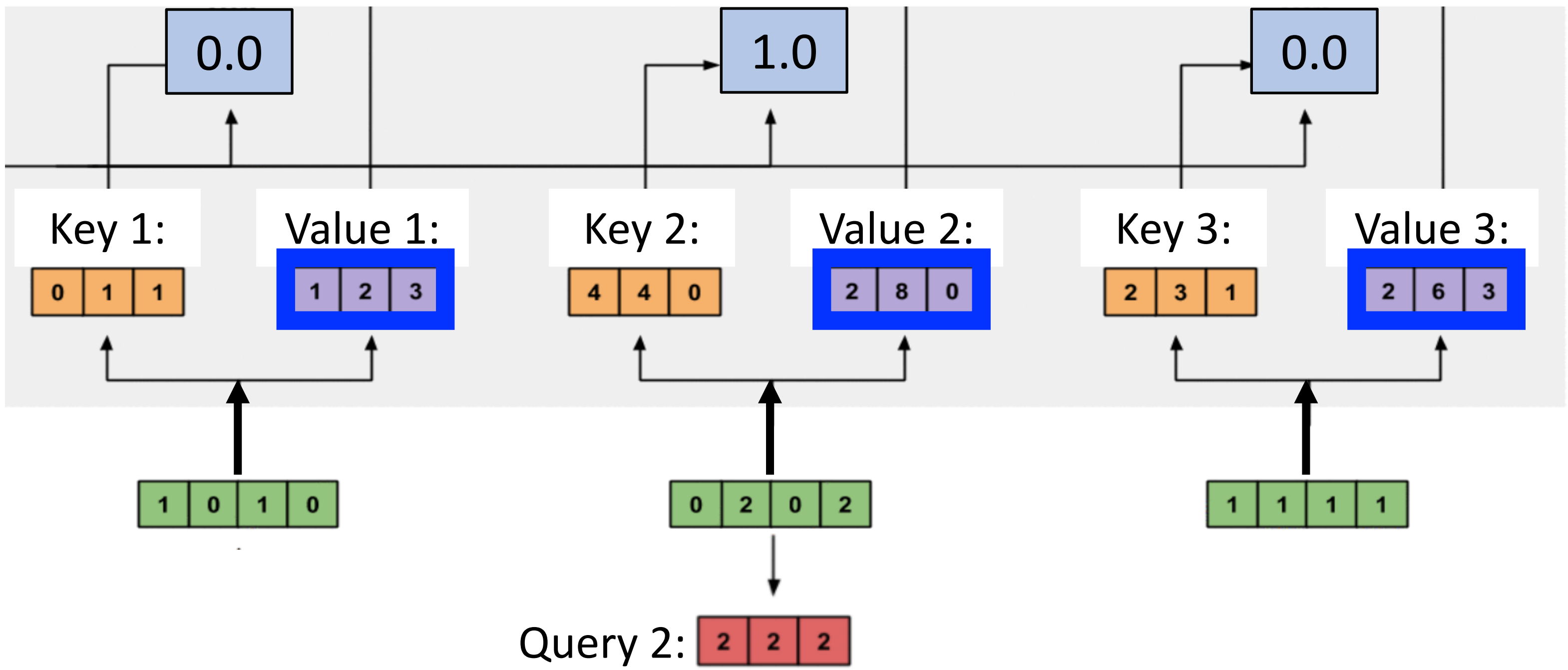
Computing Self-Attention: Example

1. Compute attention weights
- Softmax resulting 3 scores from query x keys

2. Compute weighted sum of values using attention scores



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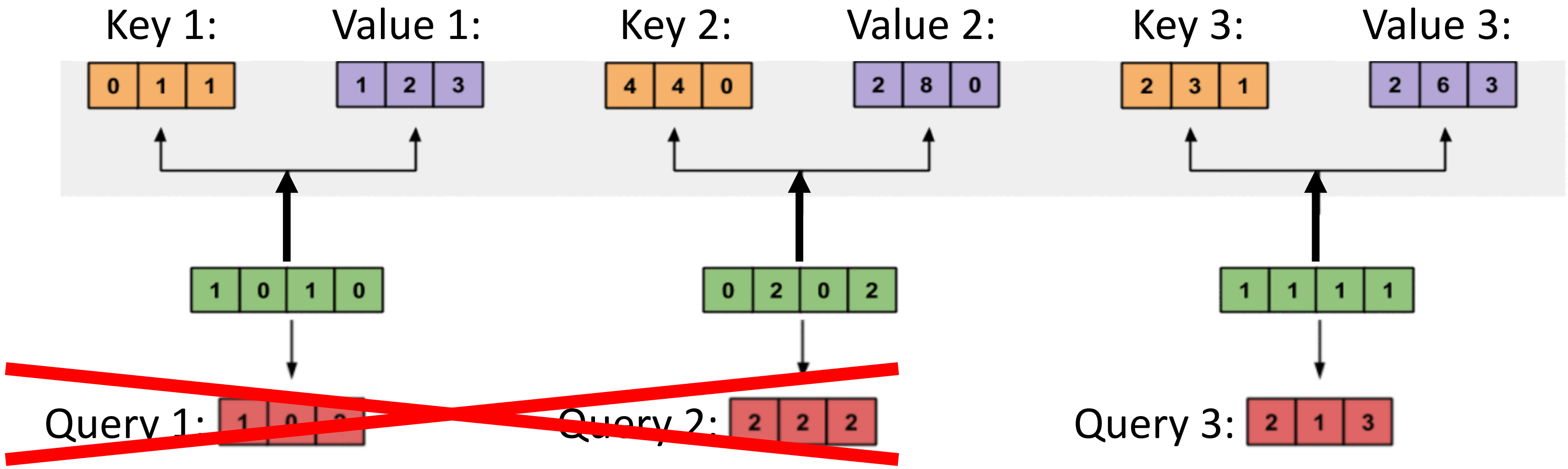

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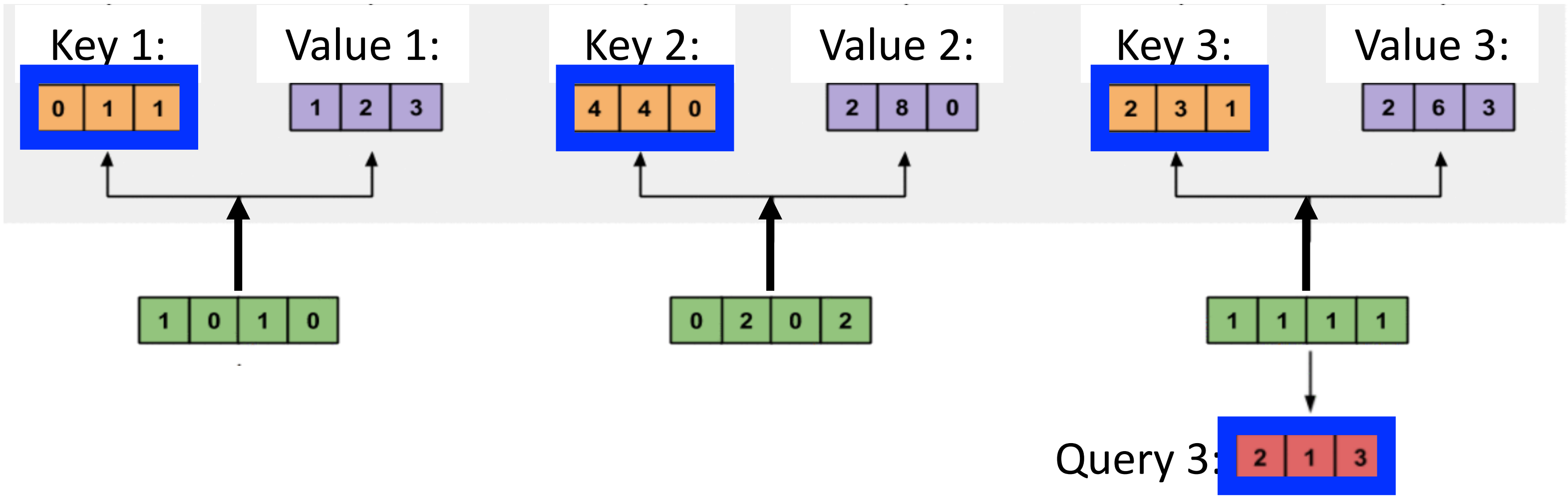
Computing Self-Attention: Example

1. Compute attention weights
- Softmax resulting 3 scores from query x keys

To which input(s) is input 3 most related?



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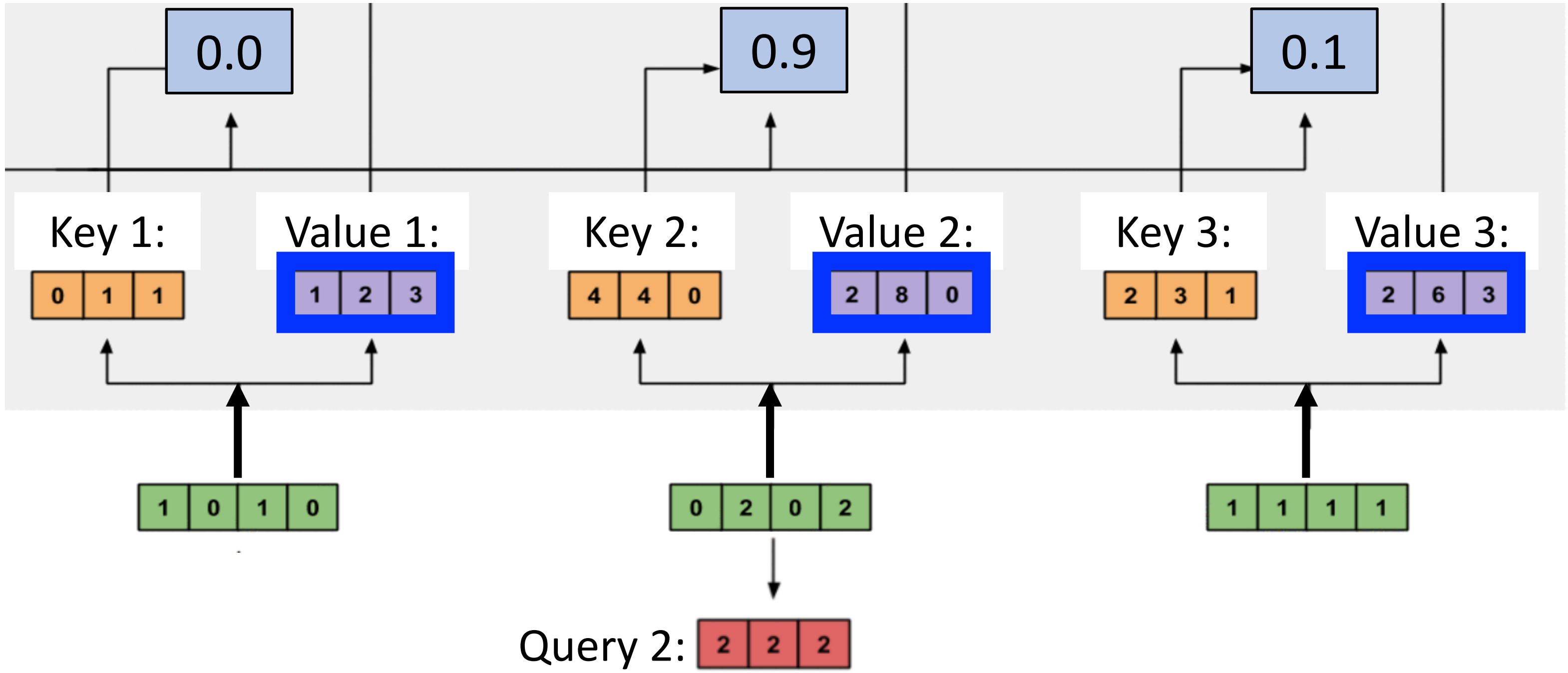
Computing Self-Attention: Example

1. Compute attention weights
- Softmax resulting 3 scores from query x keys

2. Compute weighted sum of values using attention scores



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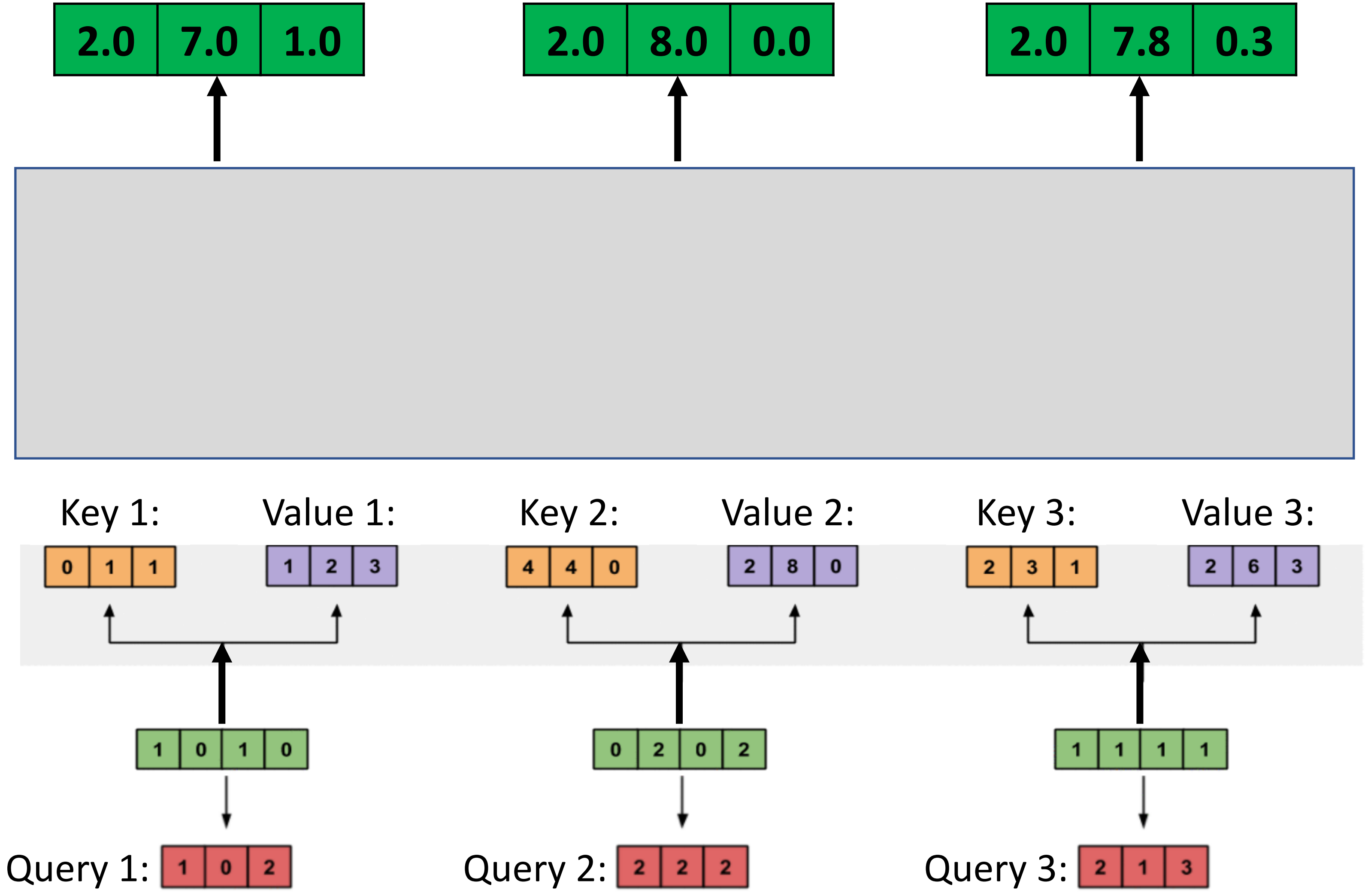
Computing Self-Attention: Example



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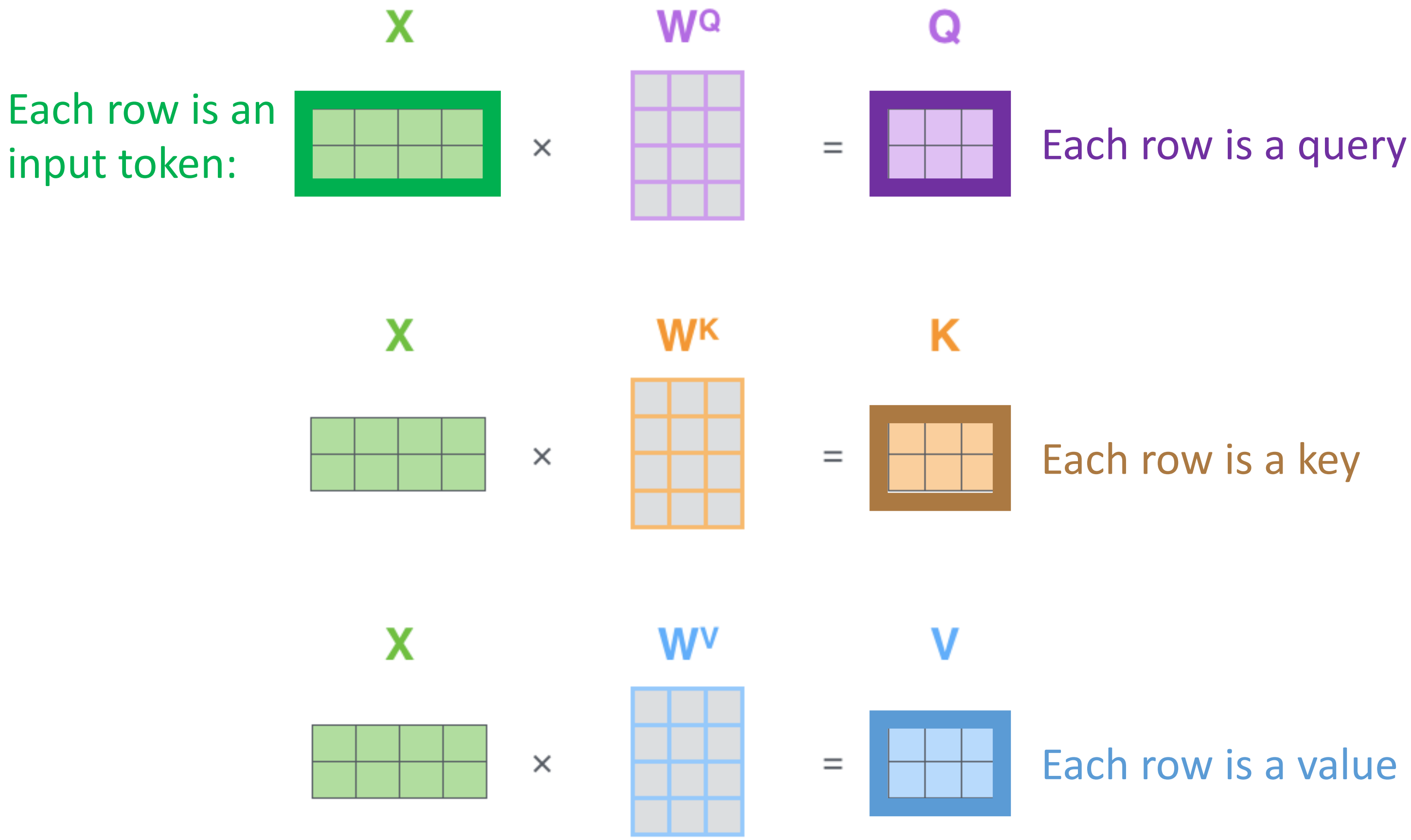
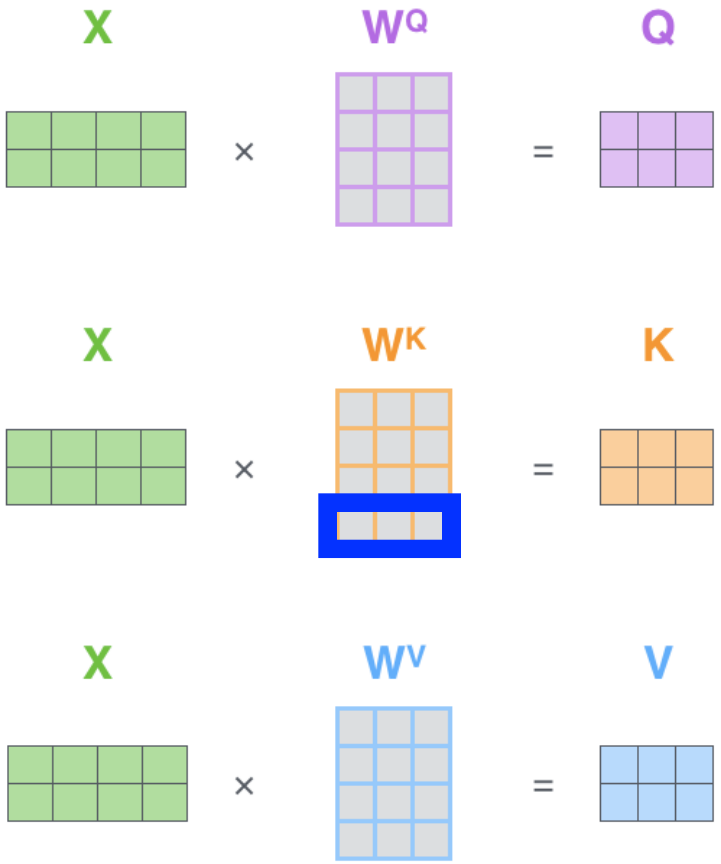
Efficient Computation for Self-Attention

Step 1

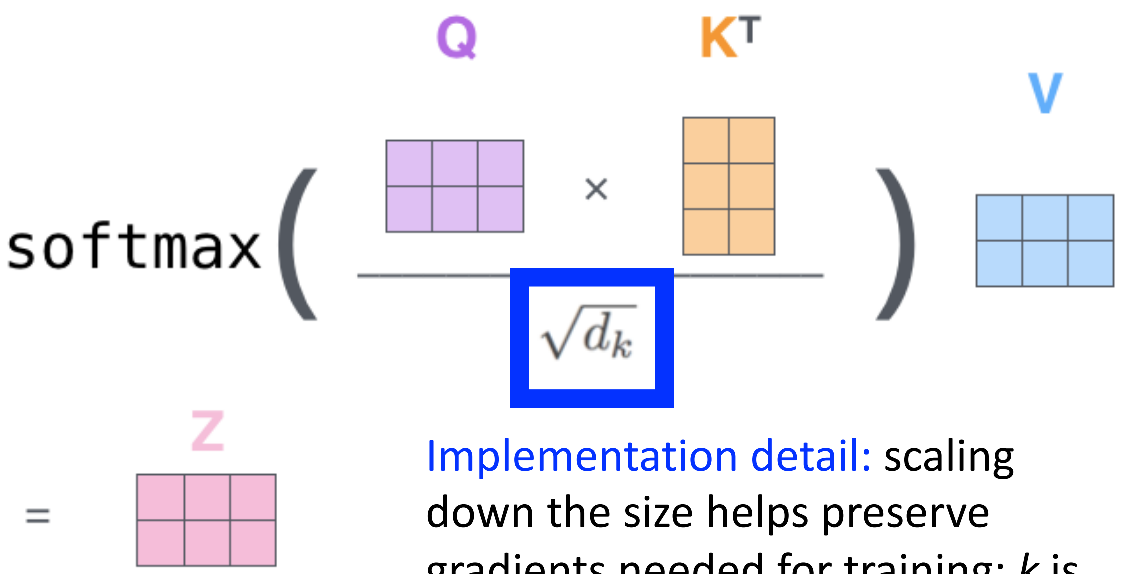


Efficient Computation for Self-Attention

Step 1



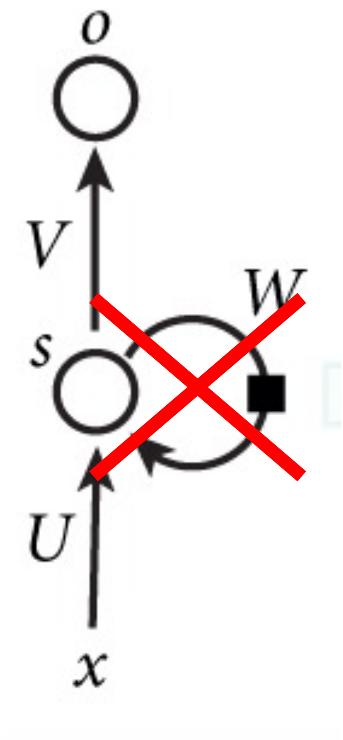
Step 2



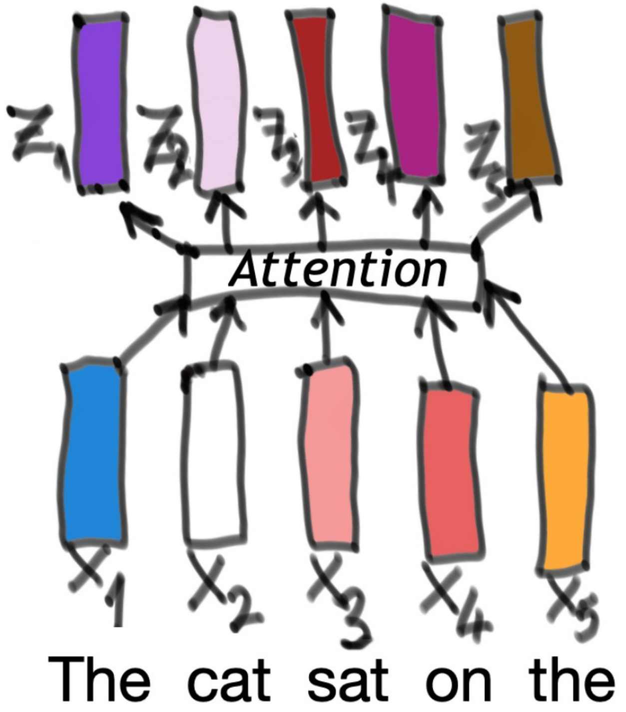
Implementation detail: scaling down the size helps preserve gradients needed for training; *k* is dimensionality of the key vector

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

Self-Attention vs RNN: Propagates Information About Other Inputs Without Recurrent Units



http://www.wildml.com/2015/09/recurrent-neural-networks-tutorial-part-1-introduction-to-rnns/



https://towardsdatascience.com/self-attention-5b95ea164f61

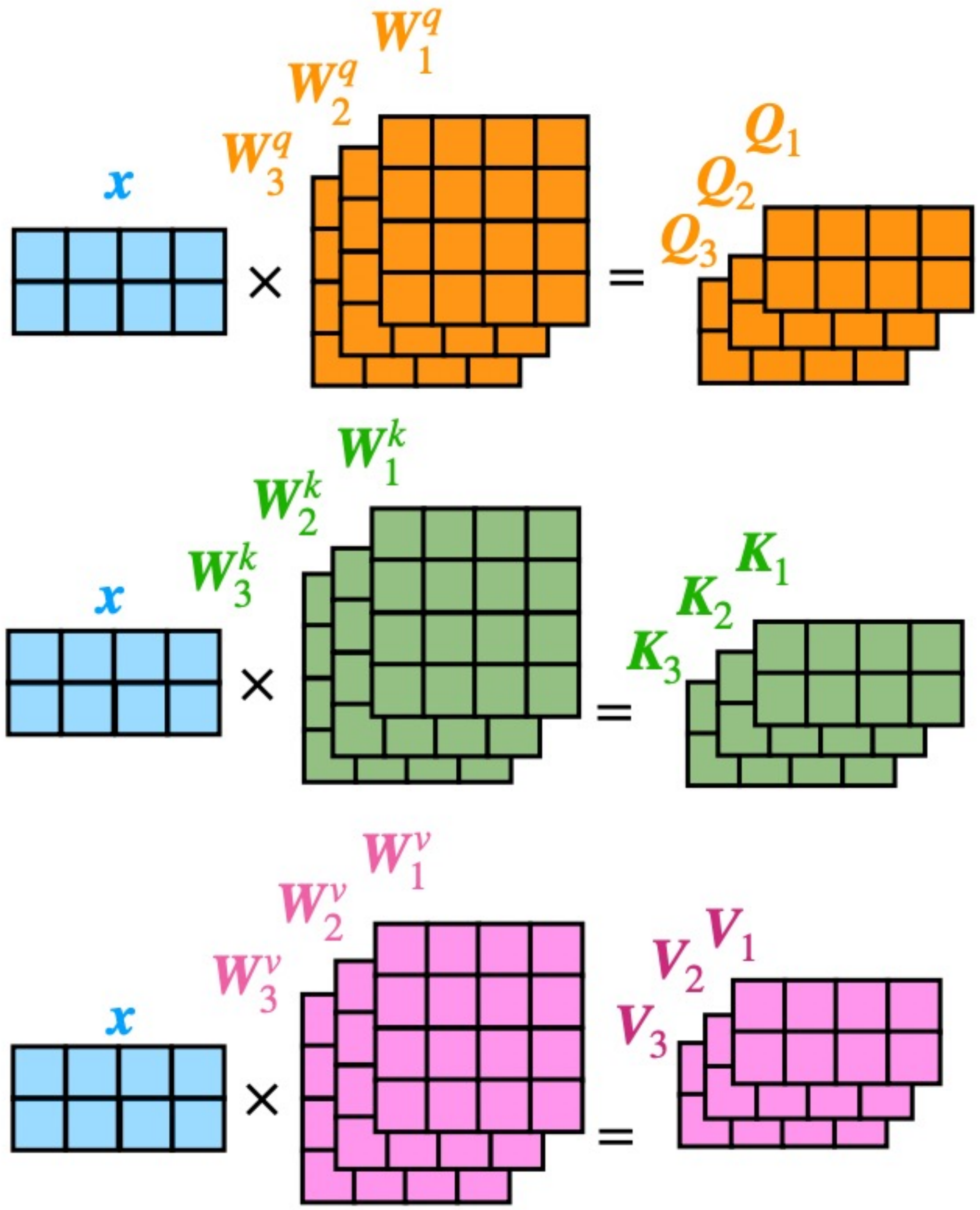
Today’s Topics

- Transformer overview
- Self-attention
- Multi-head attention
- Common transformer ingredients
- Pioneering transformer: machine translation
- Programming tutorial

Multi-head Attention

- **Goal**: enable each token to relate to other tokens in multiple ways

- **Key idea**: multiple self-attention mechanisms, each with their own key, value and query matrices



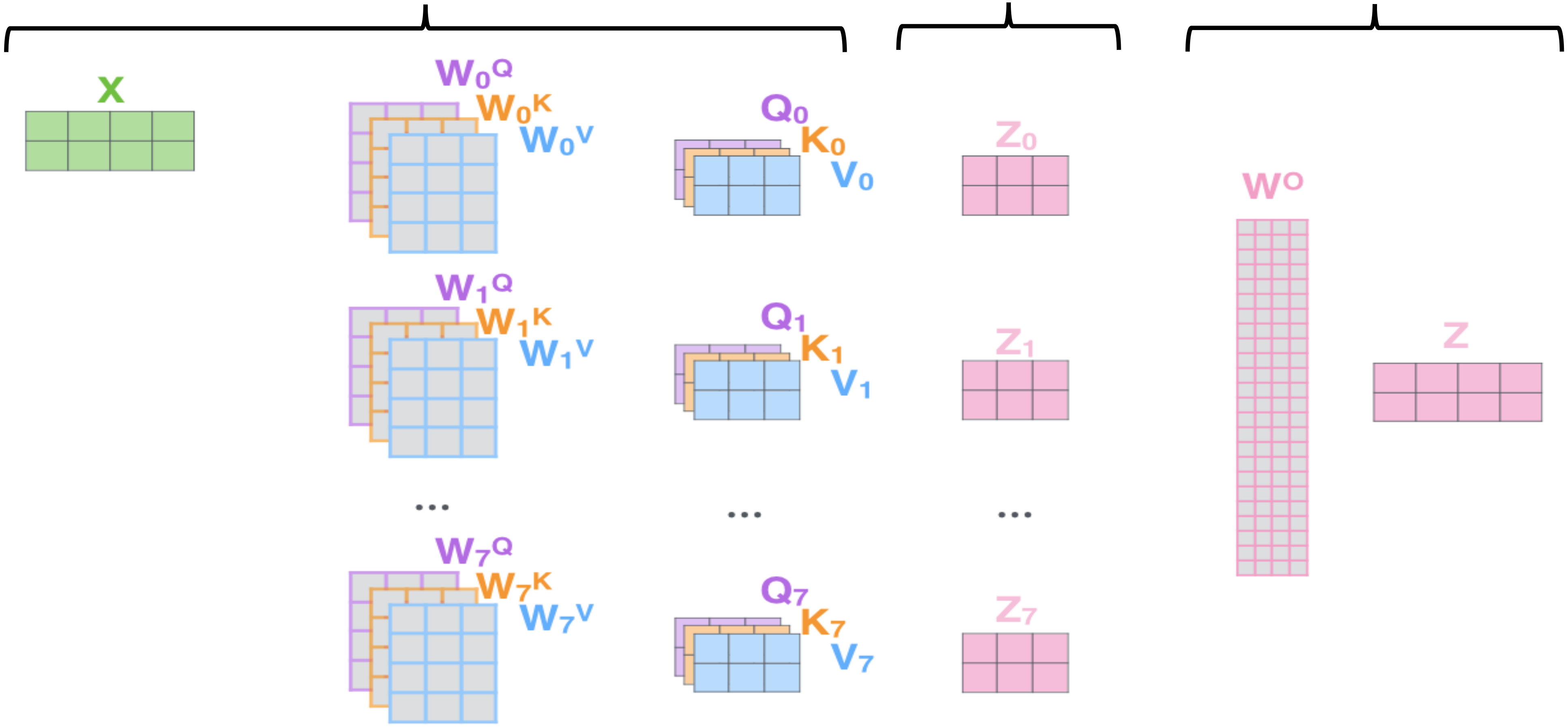
https://sebastianraschka.com/pdf/lecture-notes/stat453ss21/L19_seq2seq_rnn-transformers__slides.pdf

Multi-head Attention

1) Create query, key, and value vectors for all attentions heads

2) Compute new input representations

3) Condense all representations into a single representation by concatenating **z**-s and multiplying by a weight matrix



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Trained Multi-head Attention Examples

Figure shows two columns of attention weights for the first two attention heads

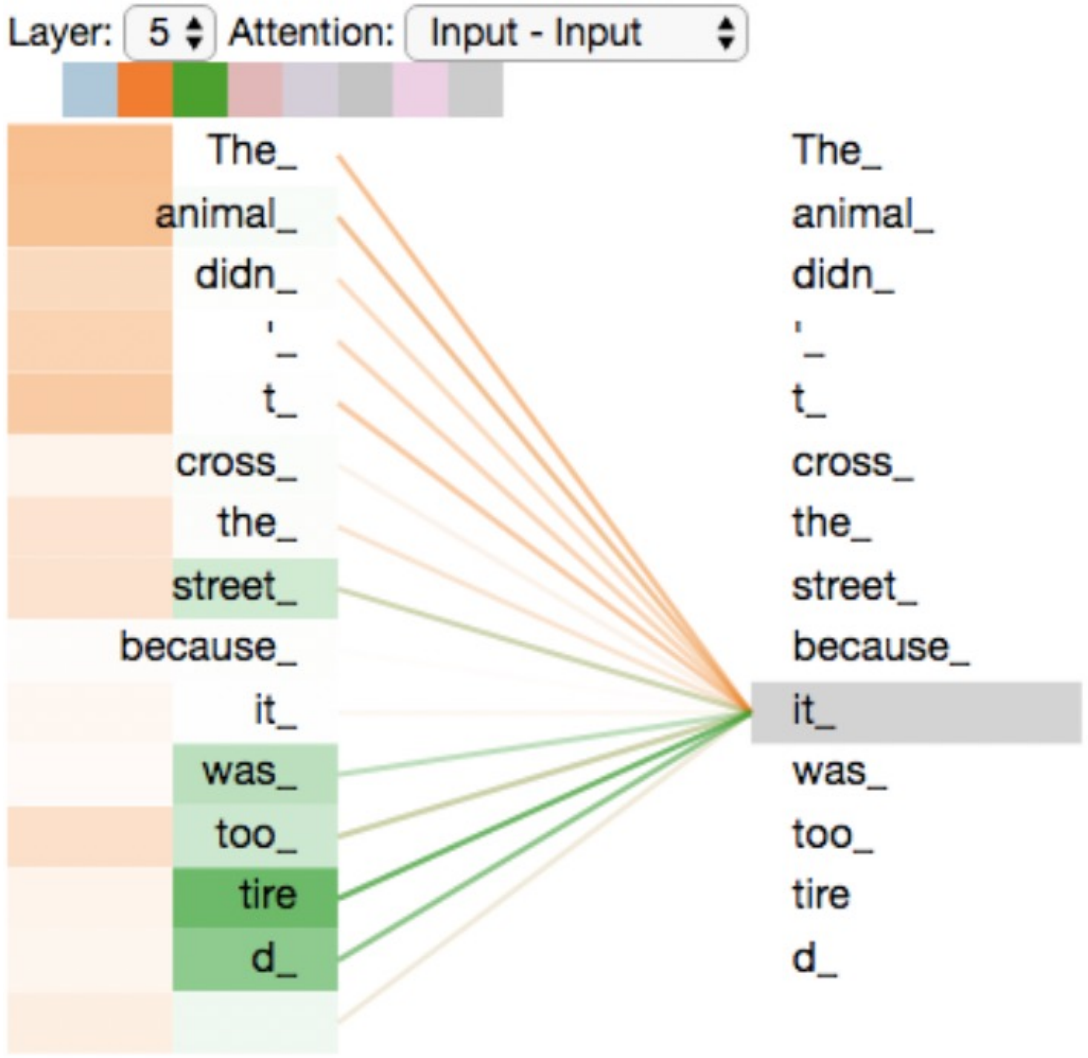
- Darker values signify larger attention scores

What does “it” focus on most in the first attention head?

- The animal (e.g., represents what is “it”)

What does “it” focus on most in the second attention head?

- tired (e.g., represents how “it” feels)



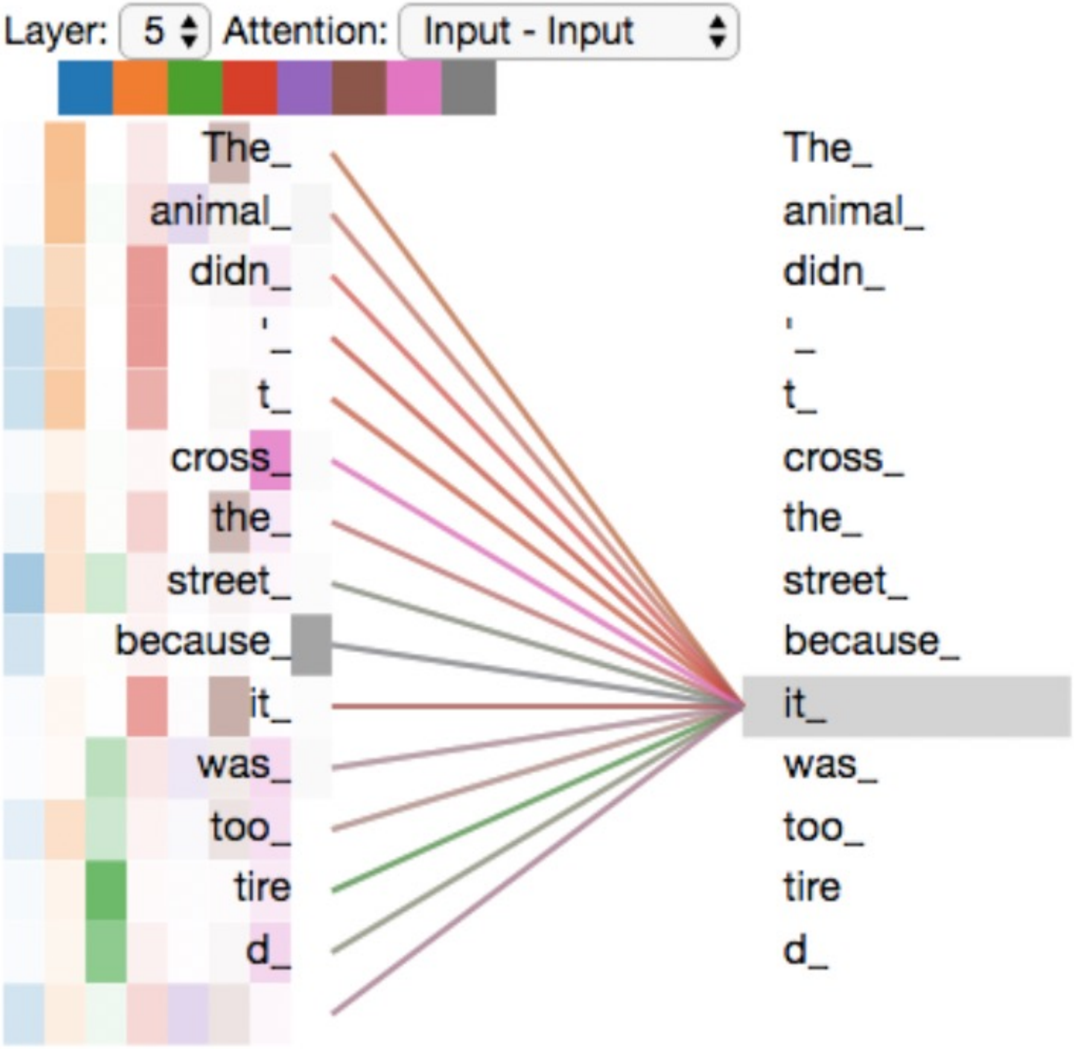
http://jalammar.github.io/illustrated-transformer/

Trained Multi-head Attention Examples

Figure shows five columns of attention weights for five attention heads

- Darker values signify larger attention scores

Attention weights may be hard to interpret



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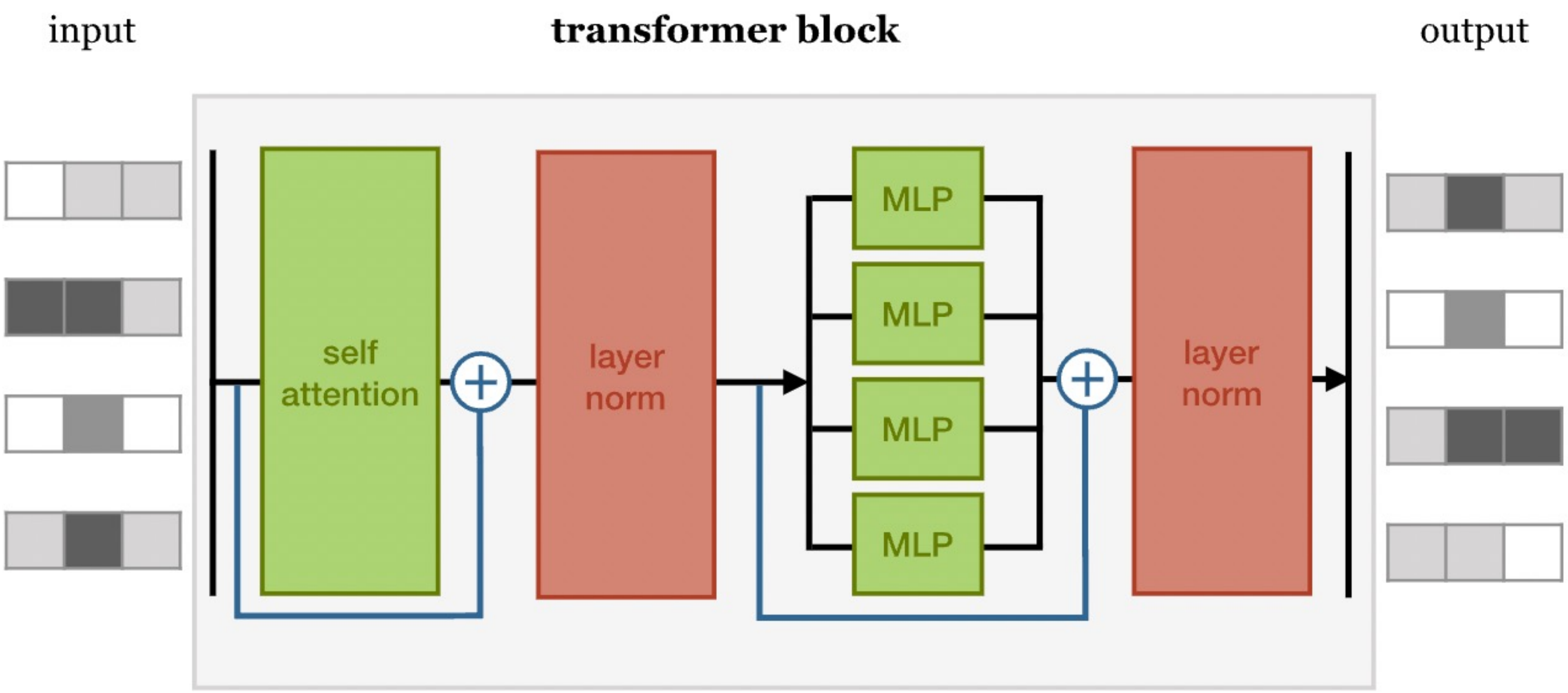
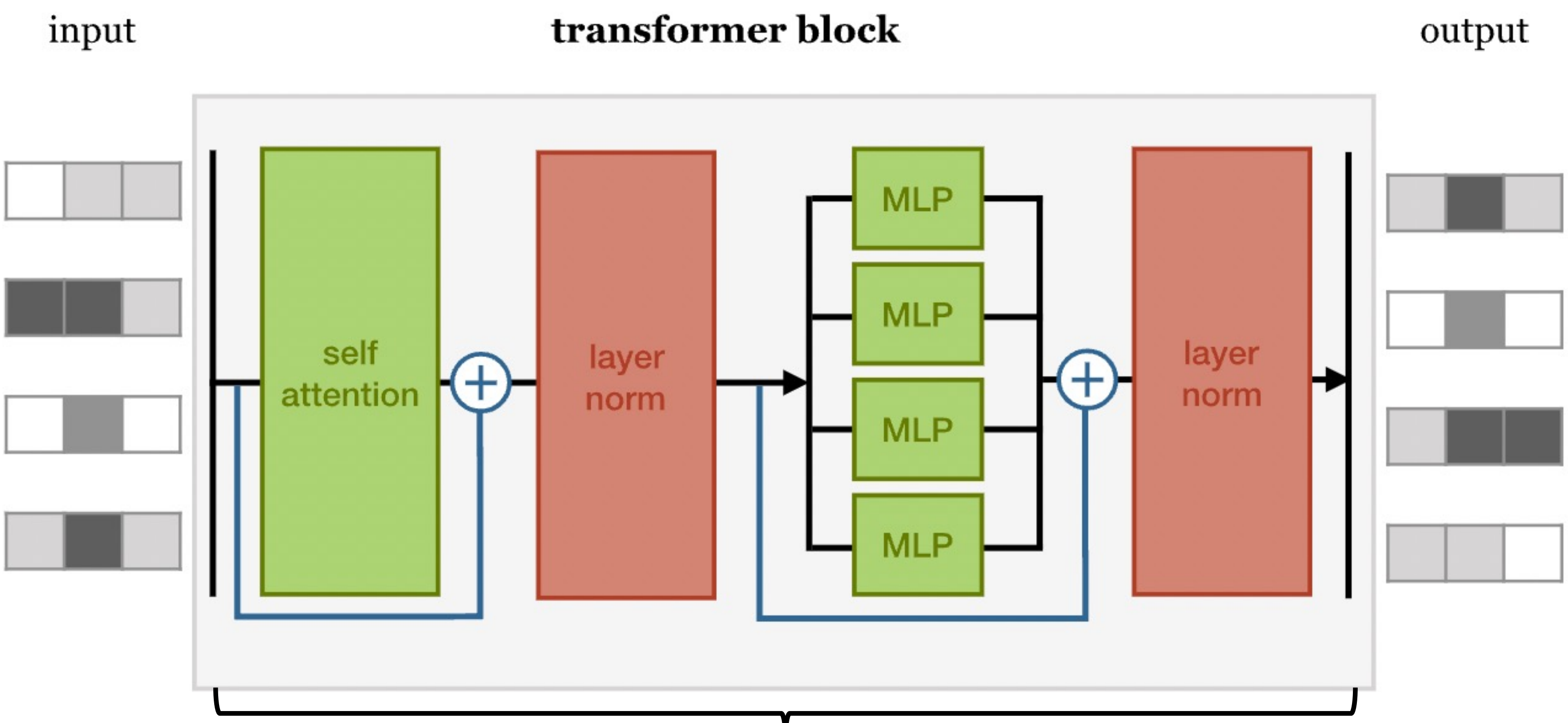
Typical Transformer Block



Architectures often chain together multiple transformer blocks, like that shown here

http://peterbloem.nl/blog/transformers

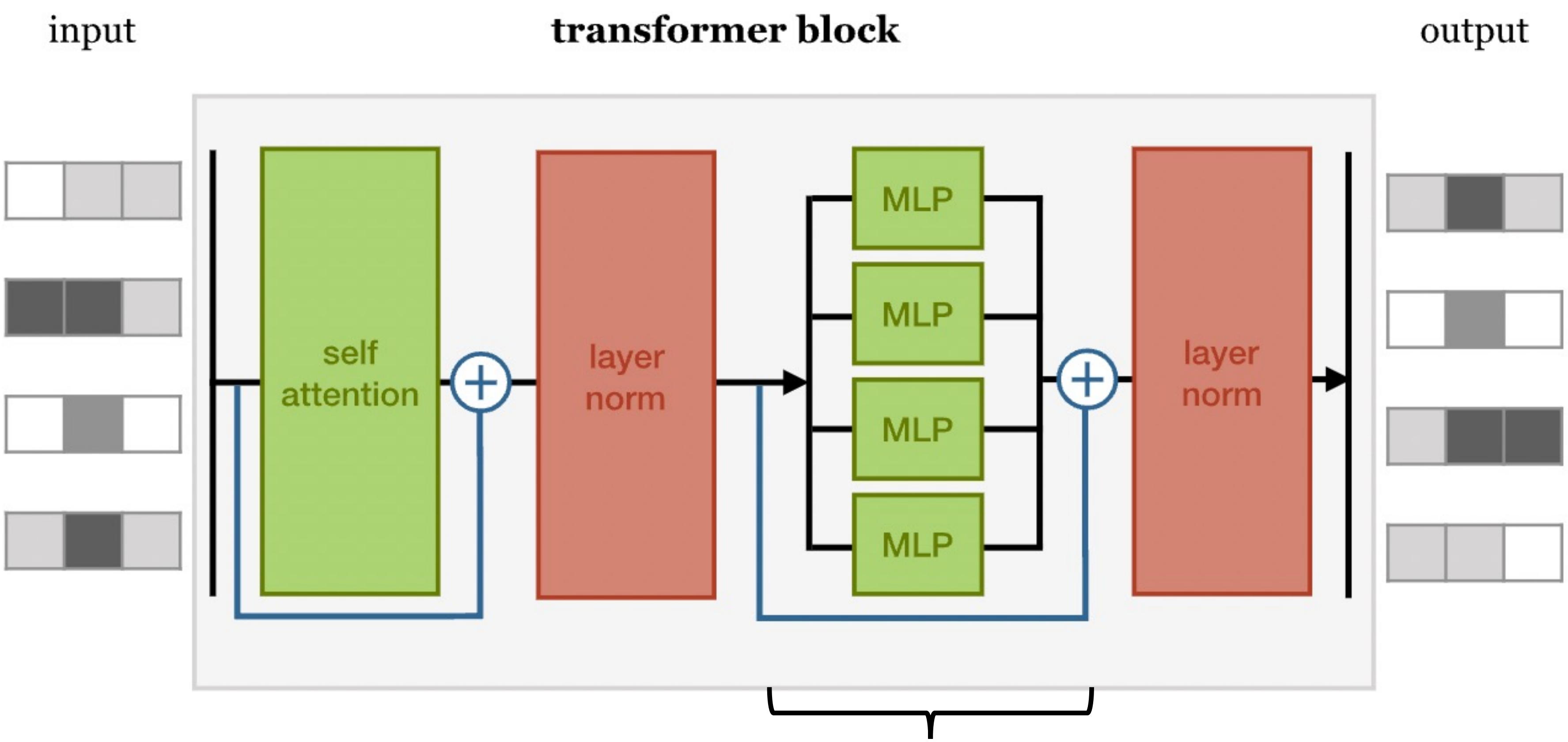
Typical Transformer Block



Layer normalization and residual connections improve training (i.e., faster and better results)

http://peterbloem.nl/blog/transformers

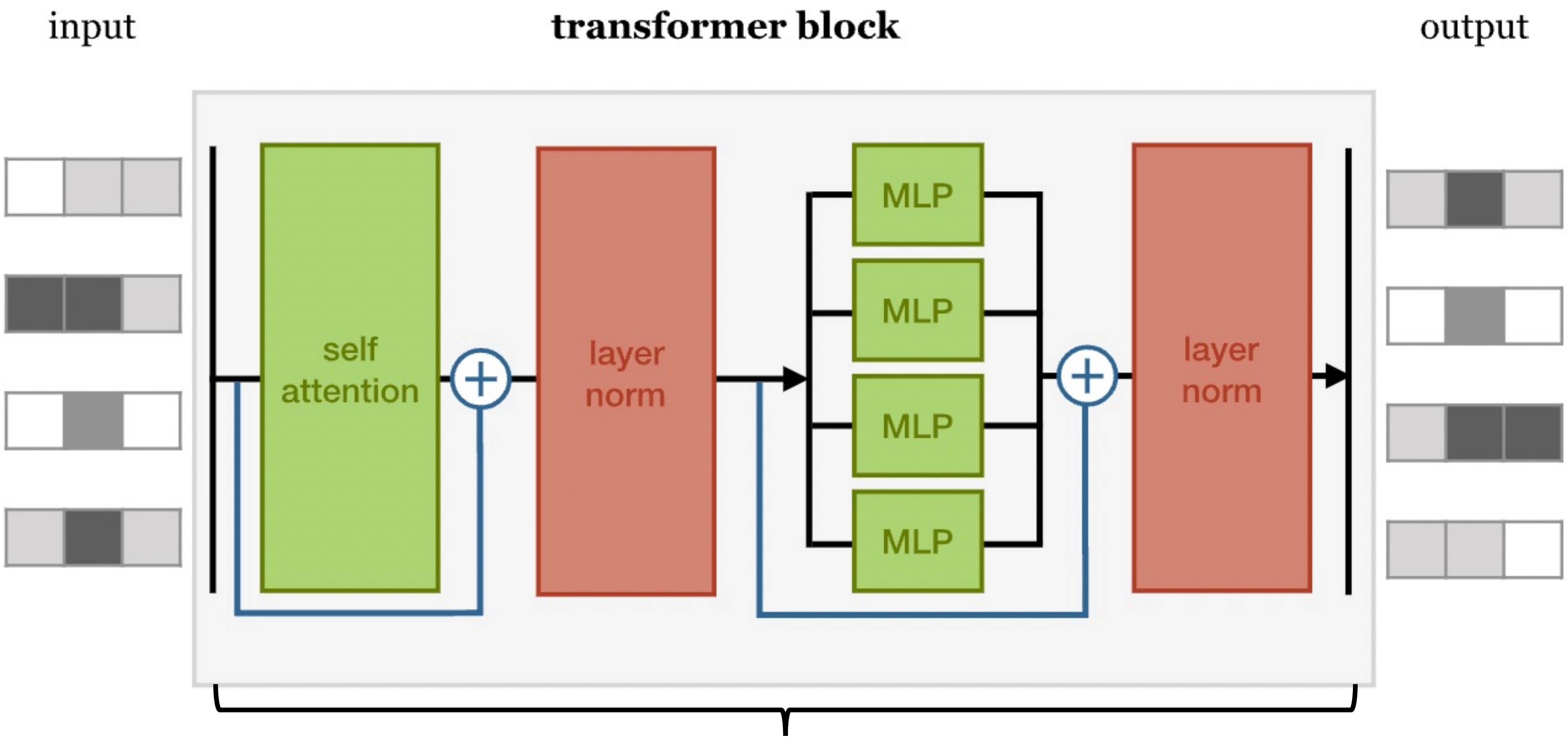
Typical Transformer Block



Feedforward layer per input

http://peterbloem.nl/blog/transformers

Typical Transformer Block



Where are non-linearities introduced in this block?

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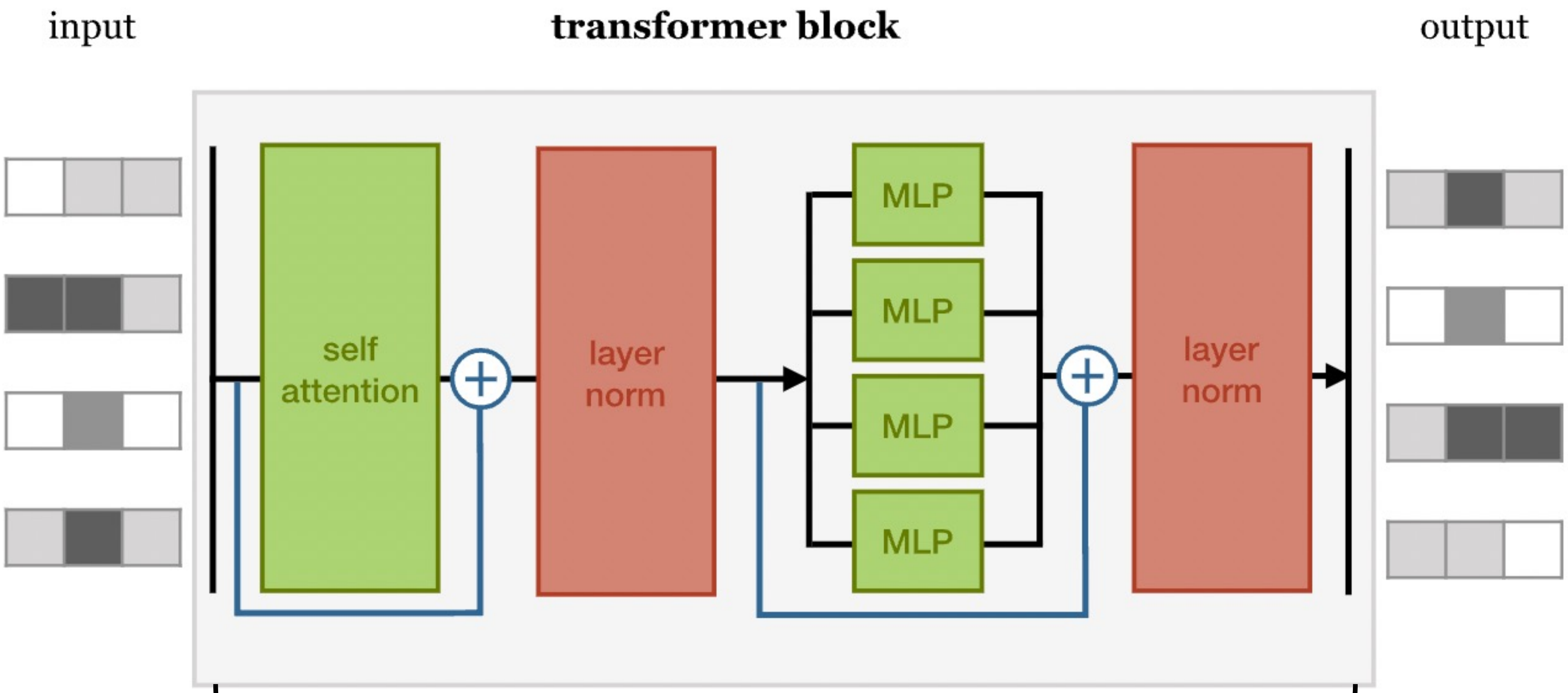
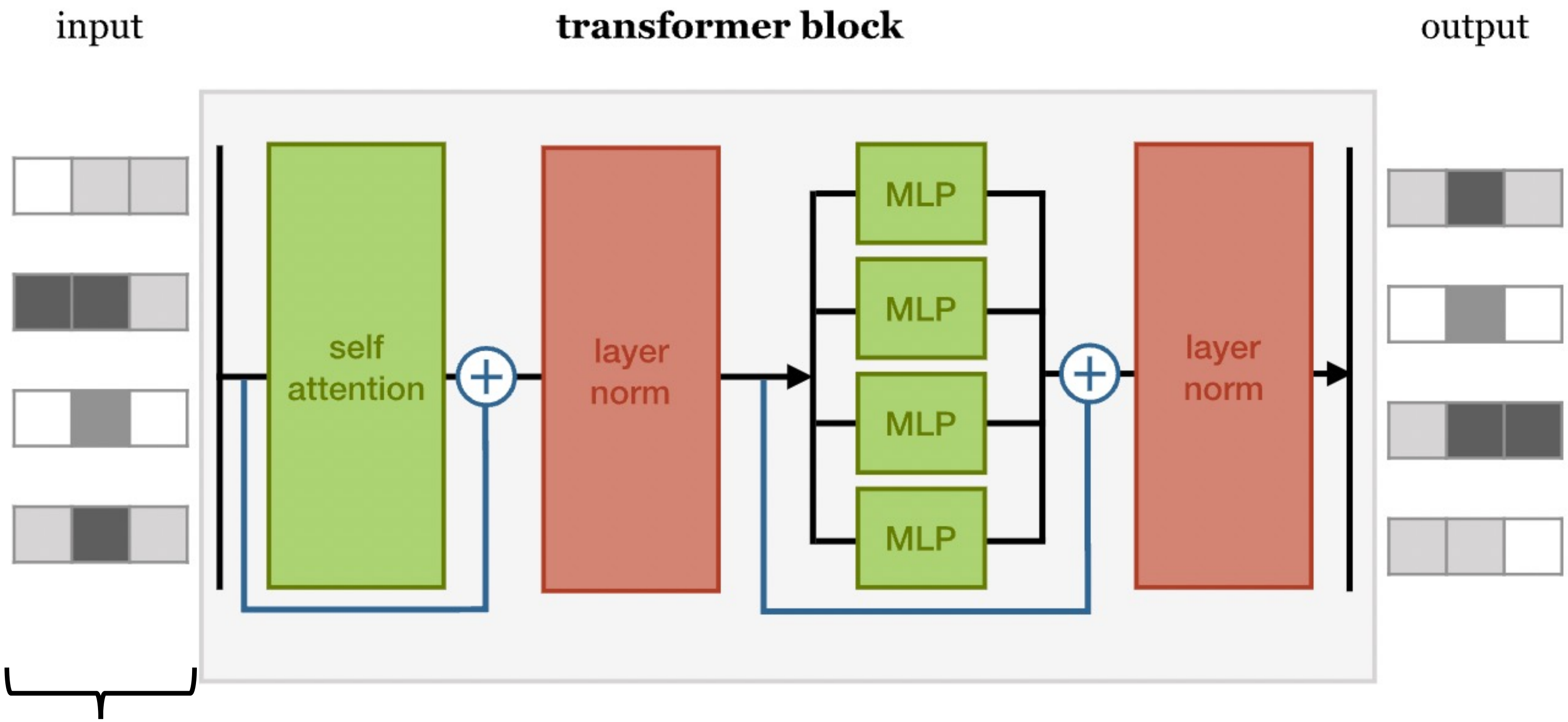
Typical Transformer Block



Non-linearities introduced in the softmax of self-attention, activation functions in MLP, and layer norms

http://peterbloem.nl/blog/transformers

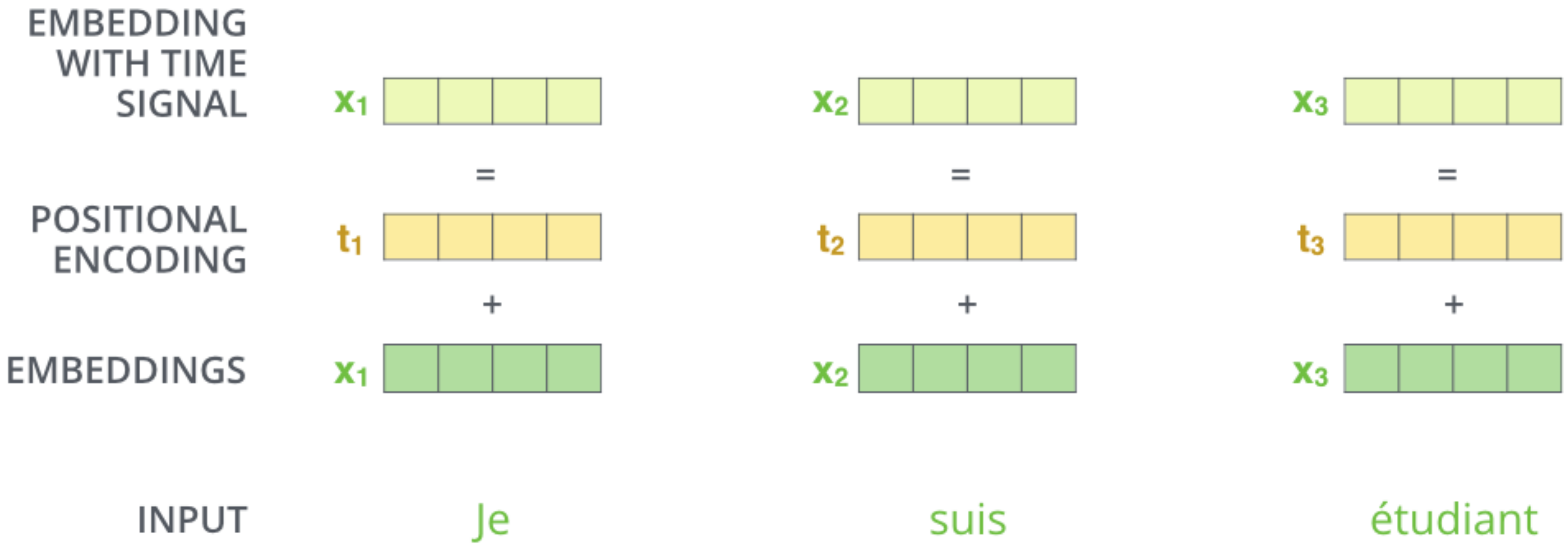
Challenge: Transformers Lack Sensitivity to the Order of the Input Tokens



Input observed as a *set* and so shuffling the order of input tokens results in the same outputs except in the same shuffled order (i.e. self-attention is *permutation equivariant*)

http://peterbloem.nl/blog/transformers

Solution: Add Position as Input to Transformer



- Options:
  - **Position embeddings**: created by training with sequences of every length during training
  - **Position encodings**: a function mapping positions to vectors that the network learns to interpret (enables generalization to lengths not observed during training)

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Attention Is All You Need

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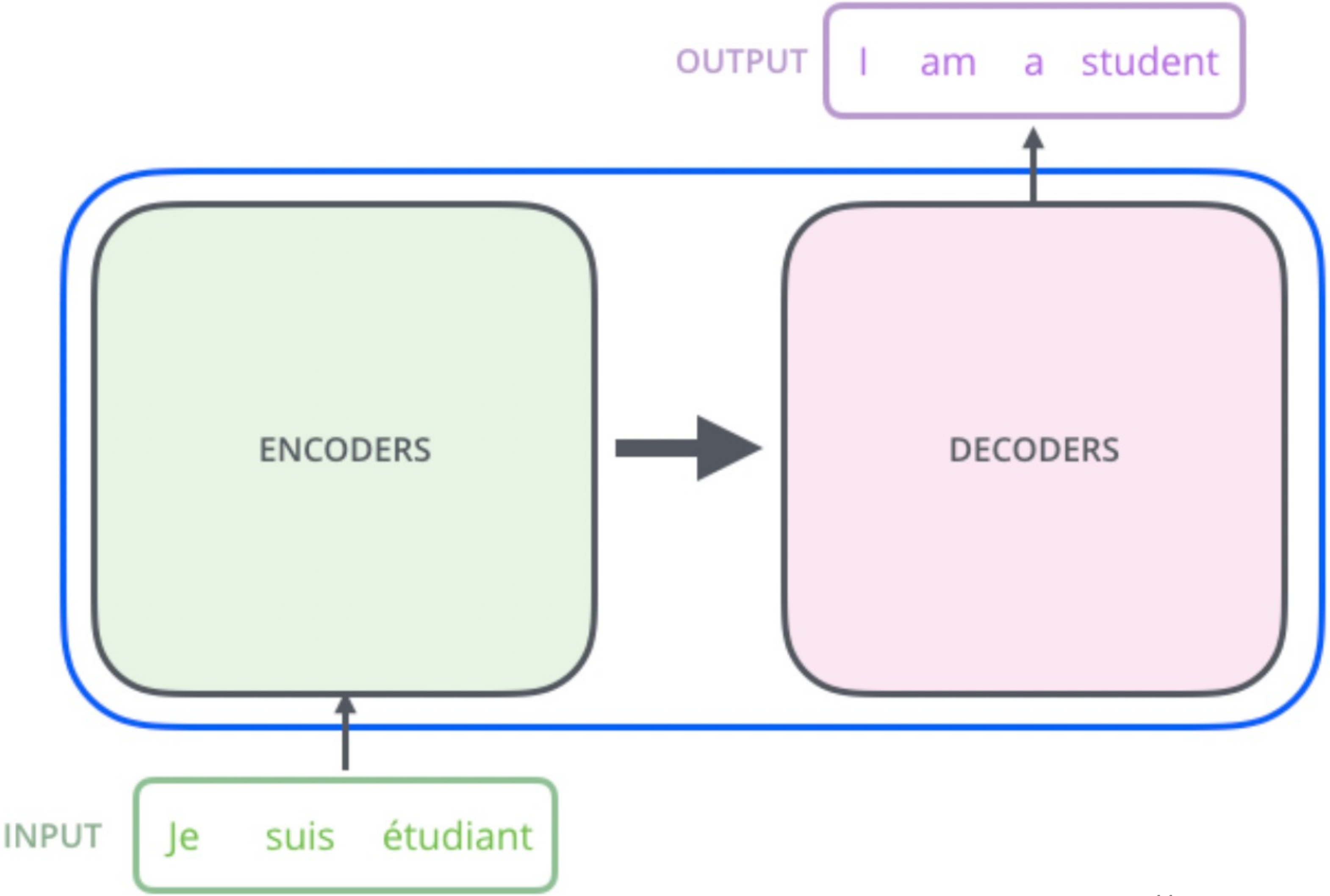
Target Application: Machine Translation



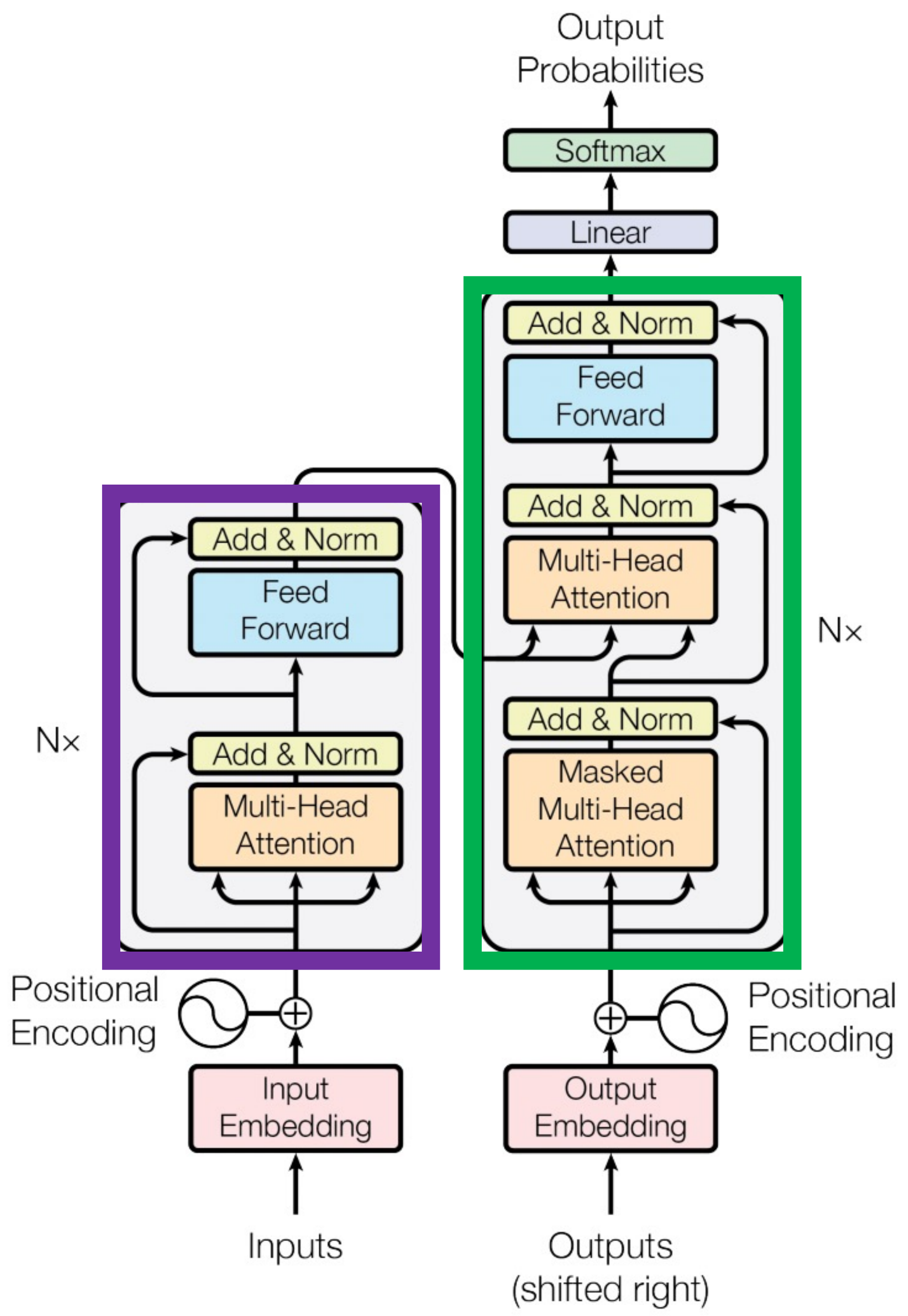
https://jalammar.github.io/illustrated-transformer/

Architecture

- Key Ingredient
  - Self-Attention in the encoder and decoder

- Other ingredients
  - Positional encoding
  - Layer normalization
  - Residual connections
  - Feed forward layers

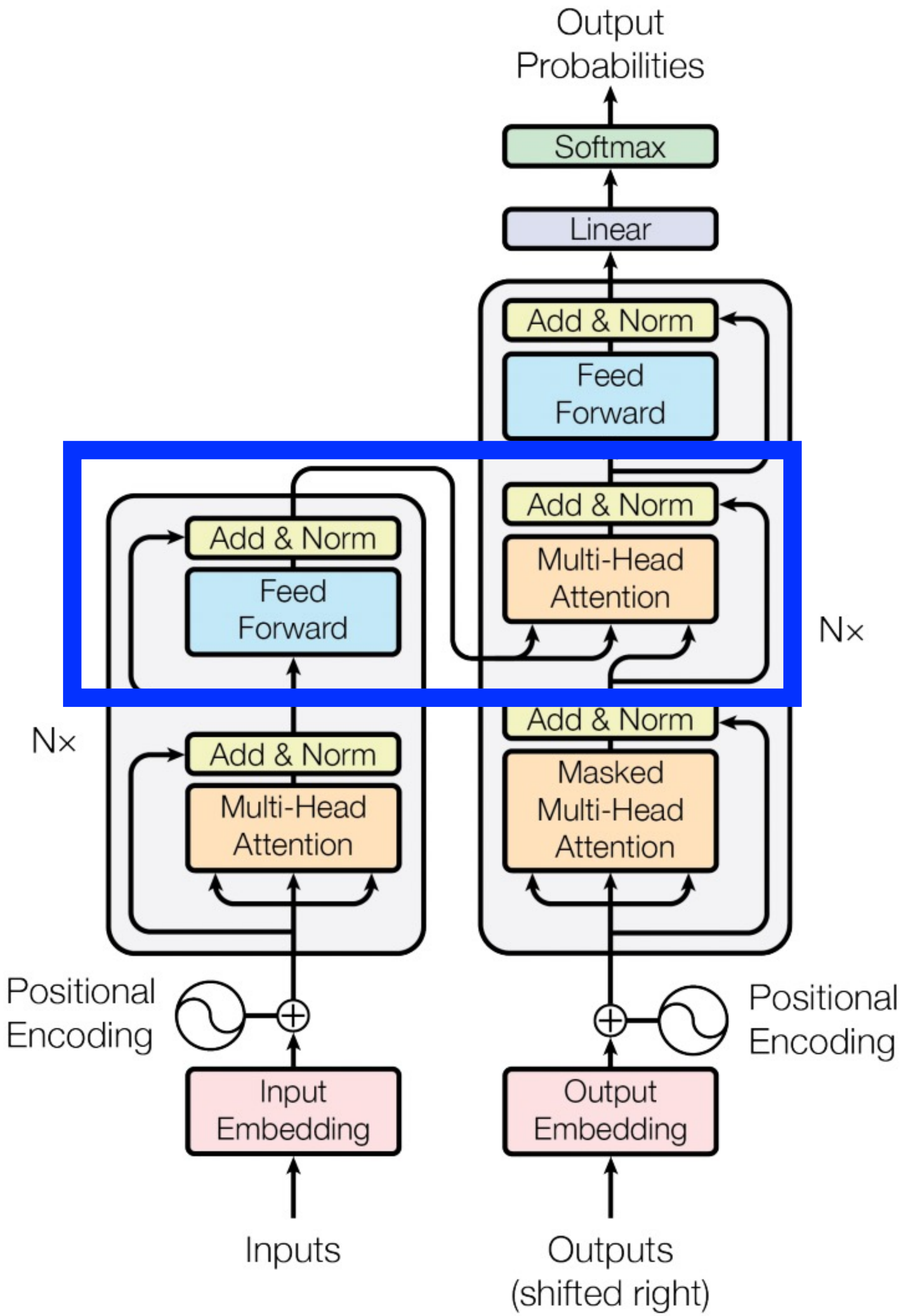
- Nx = 6 chained blocks (encoder & decoder)



Vaswani et al. Attention Is All You Need. Neurips 2017.

Architecture

The decoder performs multi-head attention on the encoder output



Vaswani et al. Attention Is All You Need. Neurips 2017.

Next Lecture: Transformers Without the Baggage of an Encoder-Decoder Architecture

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The End