Lecture 12: Transformers (Part 2)

Data C182 (Fall 2024). Week 07. Tuesday Oct 8th, 2024

Speaker: Eric Kim

Announcements

- HW01 due tonight! Tues Oct 8th 11:59 PM PST
  - Reminder: Homework slip day policy [link]
  - DSP students: for those with "Assignment extension" accommodation, we have already extended your due date on Gradescope.
    - If you are expecting one, but haven't received the extension, please make a private Ed post!
- HW02 ("RNNs") out!
  - Due: Thurs Oct 24th, 11:59 PM PST
  - In Colab (phew!)

Announcements

- Reminder: Midterm is coming up!
  - Tuesday, October 22th 2024, 6:30 PM - 8 PM.
  - Location: ~50% in 10 Evans, ~50% in Physics 1
    - We'll send exam room assignments to students shortly
  - If you're unable to make this time, please contact us ASAP (make a private Ed post)
  - Midterm will cover everything from:
    - Lectures, discussions, HW01+HW02
  - In-person, paper + pencil exam.
  - **DSP**: if you need exam accommodations, please contact us ASAP (private post on Ed)

Today's lecture

- Transformers (Part 2!)
- Multi-head self attention (MHA): deep dive
- Encoders
  - Text classification, image classification

Problem setup: sequences

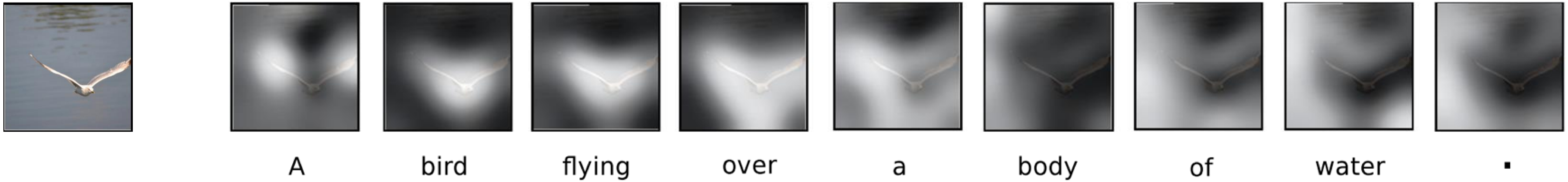
- So far: we've mainly focused on "point predictions"
  - Ex: given an image, what category is it? (CIFAR-10, from HW01!)
- Many problems are instead naturally described via sequences
  - Given a video (a sequence of audio and visual features), what is happening in the video? (action classification)
  - Given an input text sequence:
    - Generation: what should I respond with?
    - Translation: translate from English to French?
    - Classification: does this sentence have positive sentiment?

Attention

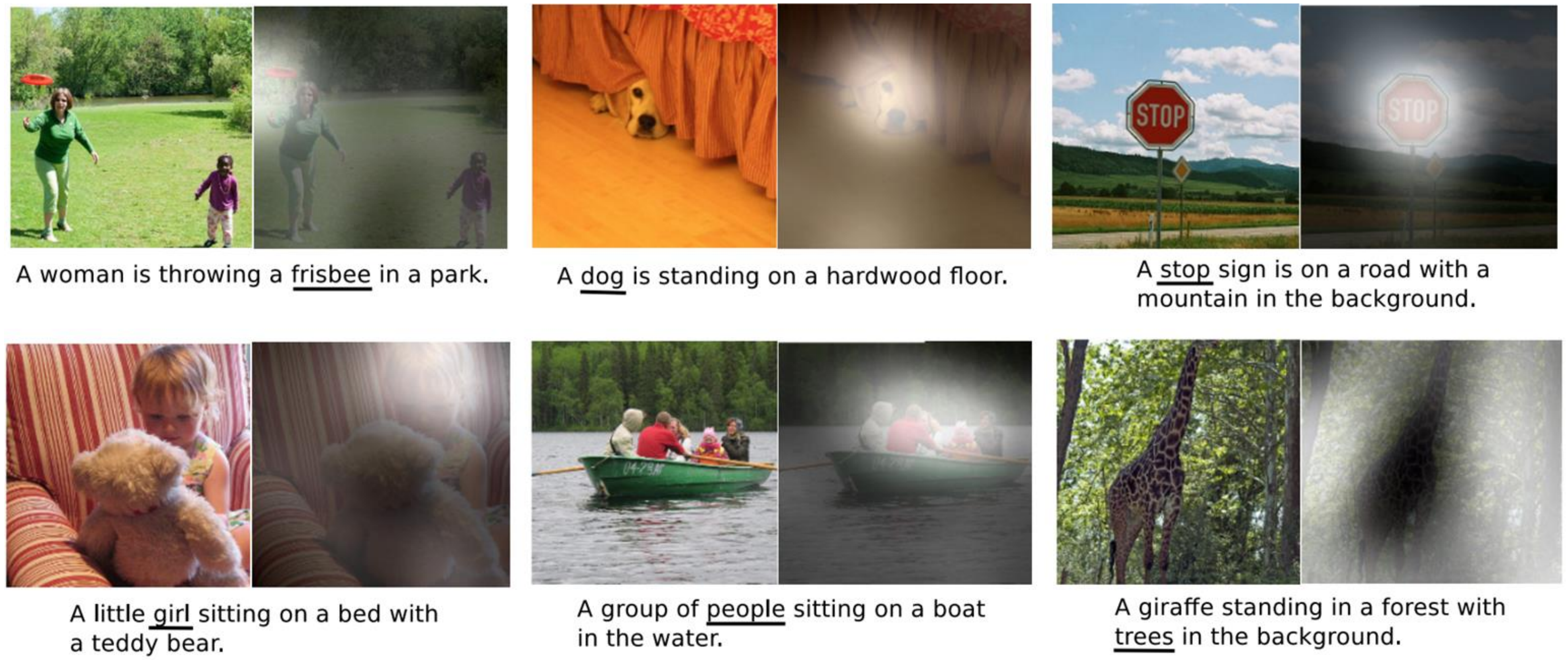
- Motivation: given an input X, when producing a prediction/output Y, we want the model to tell us "why" it returned Y
  - "Explainable AI"
- One popular approach: "Attention"
- Design your model such that the model considers certain parts of the input X more "important" than others
- Frequently visualized in papers as "attention masks"

Motivation / intuition

Observation: model learns to correlate different regions of the image with being "relevant" to a given word.



Problem setting: Image captioning.
Input: image.
Output: text caption describing the image.



Xu et al, “Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention”. ICML 2015.

"Attention Is All You Need" (2017)

- Paper that introduced the "Transformers" model architecture [link]
- Highly influential and impactful
  - Ex: powers Chat-GPT!
  - Basically, transformers is now ubiquitously used in AI/ML
- Originally focused on the text domain: machine translation, and sentence parsing ("English constituency parsing")
  - Now, transformers are used in other domains like: images, videos, user actions, etc.

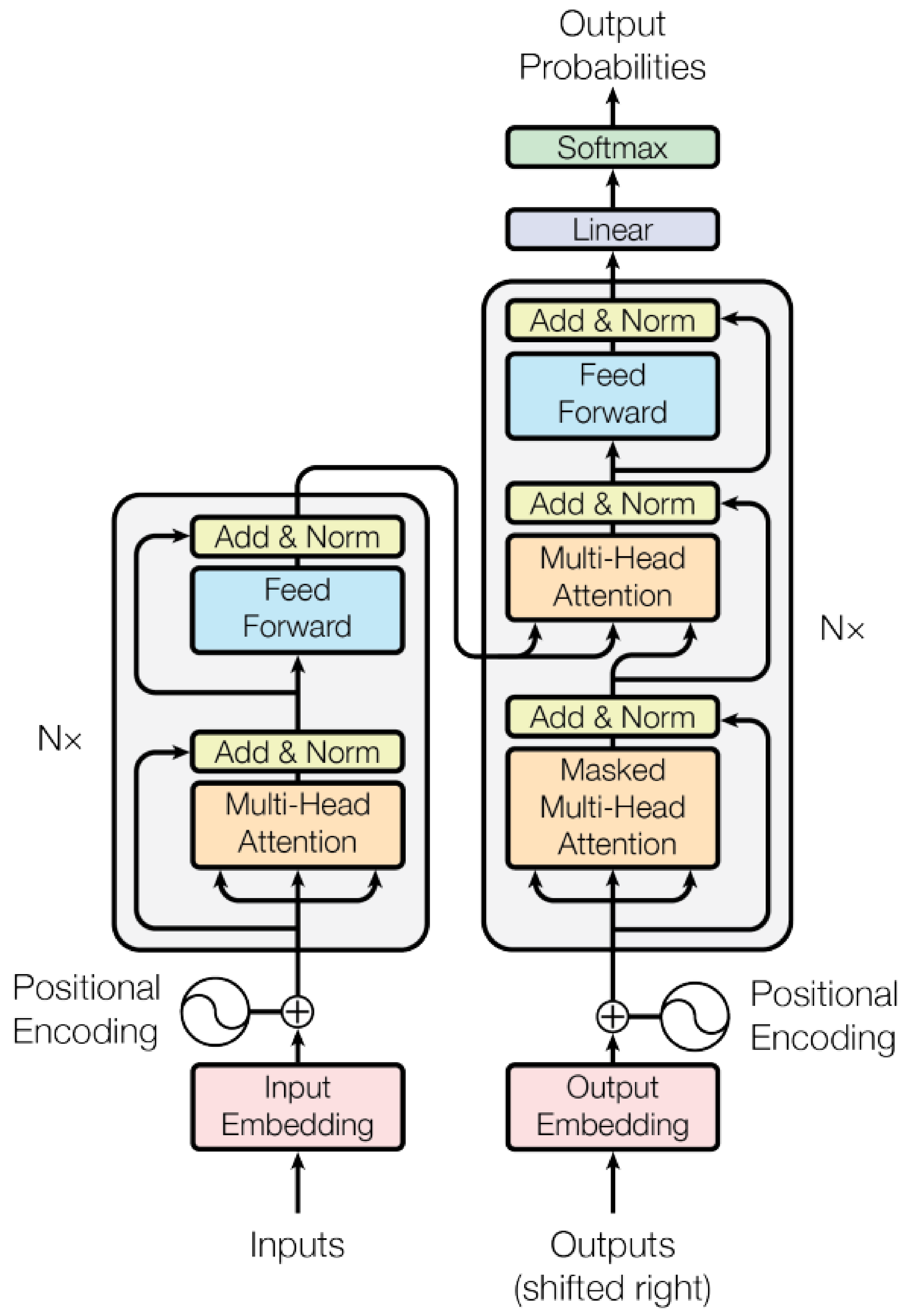


Figure 1: The Transformer - model architecture.

Multihead self attention (MHA)

- General idea: MHA layer does two things
  - (1) **Self-attention**. Learn which parts of the input are important to produce the desired prediction.
  - (2) **Attention-aware transformation**. Transform the input features in a way where the "important" parts are highlighted (attention) to learn a stronger representation.
    - Notably, MHA is good at capturing "long range" interactions, something that RNNs have historically had difficulty with

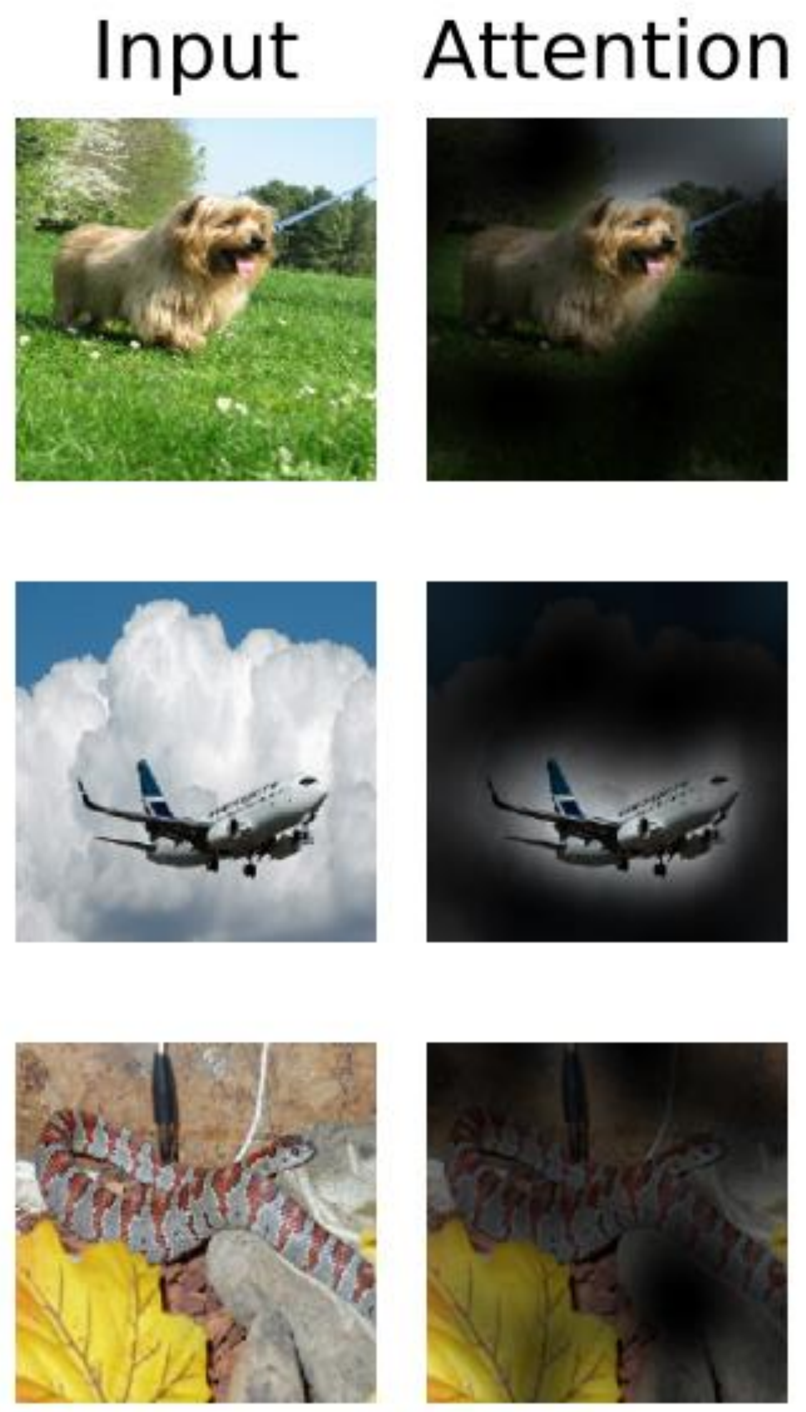


Figure 6: Representative examples of attention from the output token to the input space. See Appendix D.7 for details.

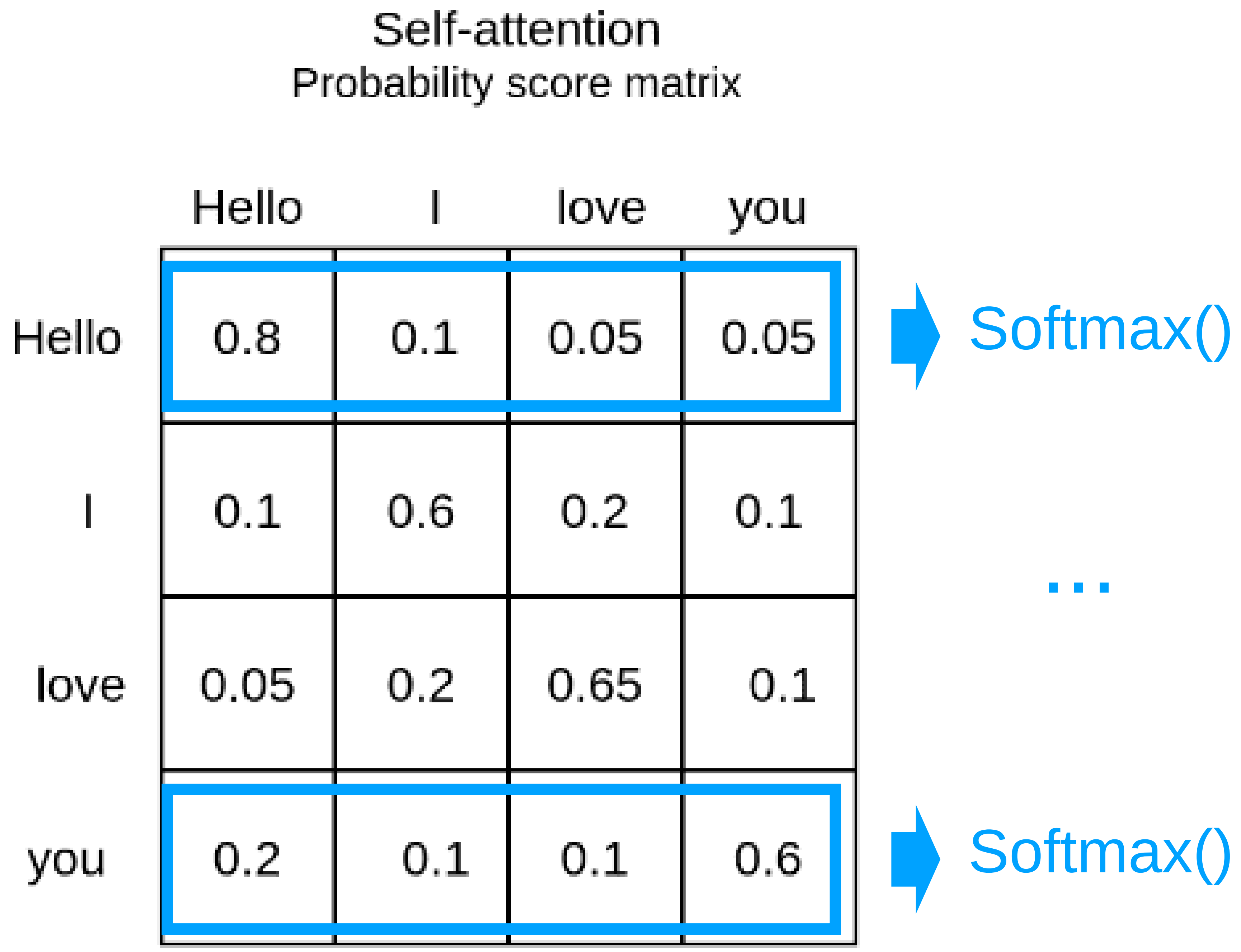
https://arxiv.org/abs/2010.11929

MHA (v0)

- Exercise: Let's build up, step-by-step, to the "full" MHA
- Note: to simplify things (somewhat), let's assume we're working with a single input sequence X, and batchsize=1 (shape=[seq_len, d]).
  - Aka we're looking at just the Encoder (more on that soon)

MHA (v0): attention scores

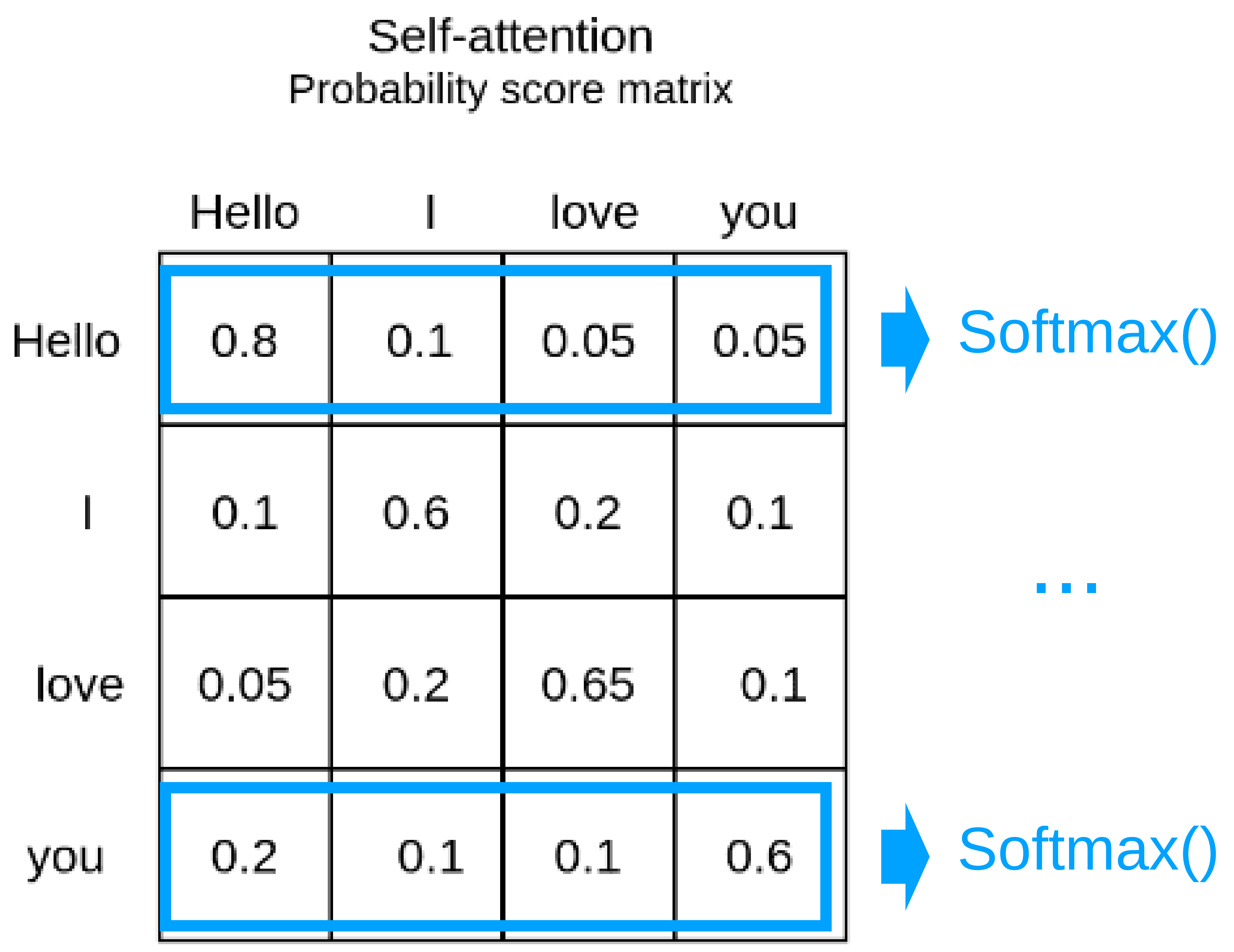
- First up: how do we compute attention scores?
- Question: given an input X with shape=[seq_len, d], what should the attention scores shape be?
  - **Answer**: [seq_len, seq_len]! Ex: attn_scores[0, 2] tells me "how important is token 2 to token 0?"
- Question: suppose I want to make the attention scores more interpretable (eg as probability scores), and have the rows of the attention scores sum to 1.0: attn_scores[0, :].sum() == 1.0. How can I achieve this?
  - **Answer**: softmax() across each row!



https://theaisummer.com/transformer/

MHA (v0): attention scores

- Question: what is the simplest way you can think of to calculate self-attention? (X shape=[seq_len, d])
  - **Answer**: one way is to multiply all pair-wise dot products between rows of X:
    - attn_scores = softmax(X * X^T, dim=1)
- Pro: simple
- Con: we're not learning anything here. What if X isn't good at calculating attention scores?
  - It's not "deep" enough...
    - Let's learn some transformations of X!



https://theaisummer.com/transformer/

MHA (v0): Query, Key, Value

Let: X be [seq_len, d]

Step 1: Calculate Query, Key, and Value:

shape=[seq_len, d]

$$\mathbf{Q} = \mathbf{X}\mathbf{W}^{(q)}$$
$$\mathbf{K} = \mathbf{X}\mathbf{W}^{(k)}$$
$$\mathbf{V} = \mathbf{X}\mathbf{W}^{(v)}$$

W^q, W^k, W^v are [d, d], and are learned linear transforms

Step 2: Use Q, K to calculate attention scores:

$$attn\_scores = softmax(\frac{QK^T}{\sqrt{d}})$$

shape=[seq_len, seq_len]

softmax is done over rows

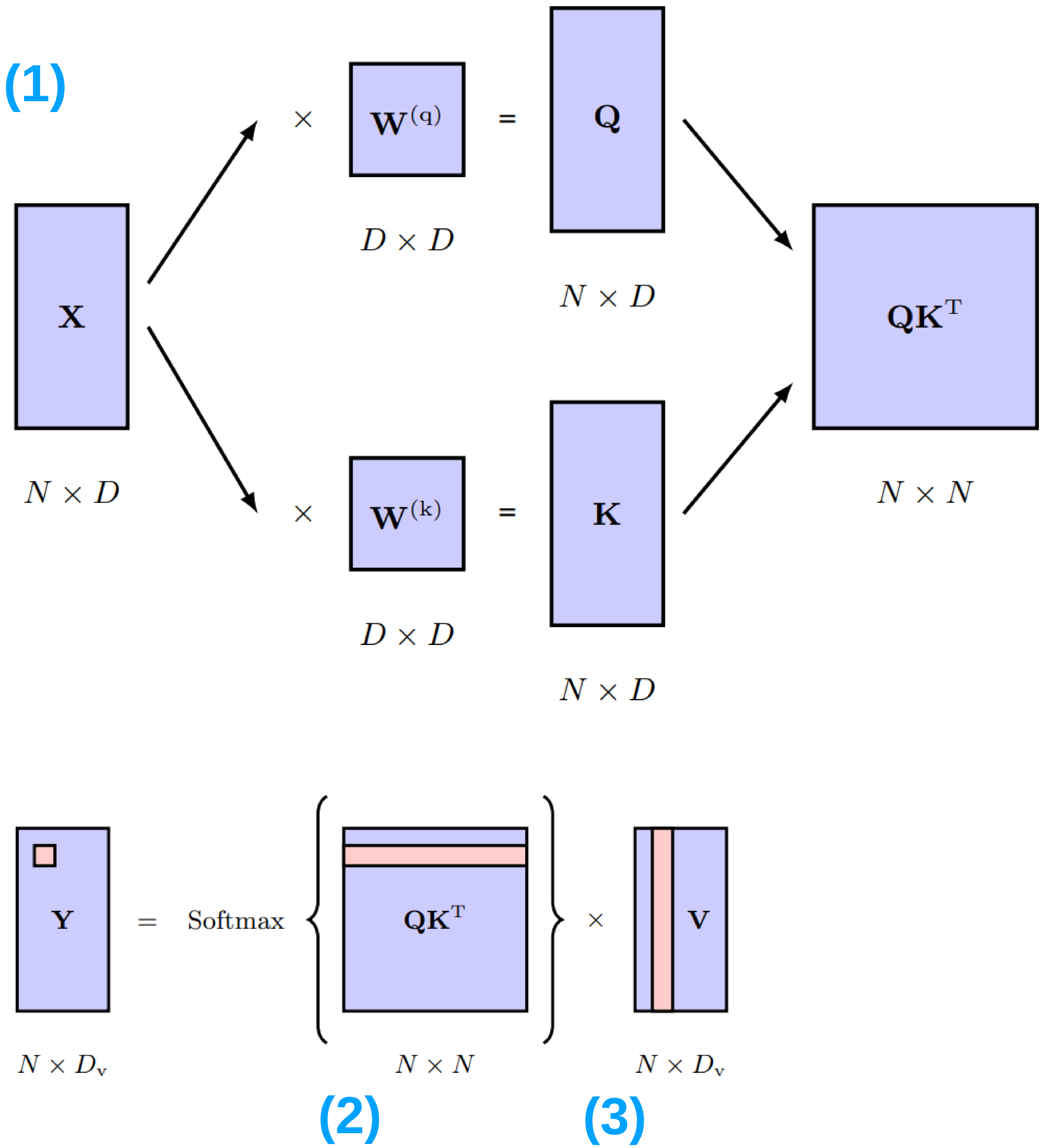
Divide by sqrt(d) to avoid issues with vanishing gradients when d is large

Step 3: Compute final MHA output

$$Y = softmax\left(\frac{QK^T}{\sqrt{d}}\right)V$$

shape=[seq_len, d]

...and repeat! Can easily stack MHA layers



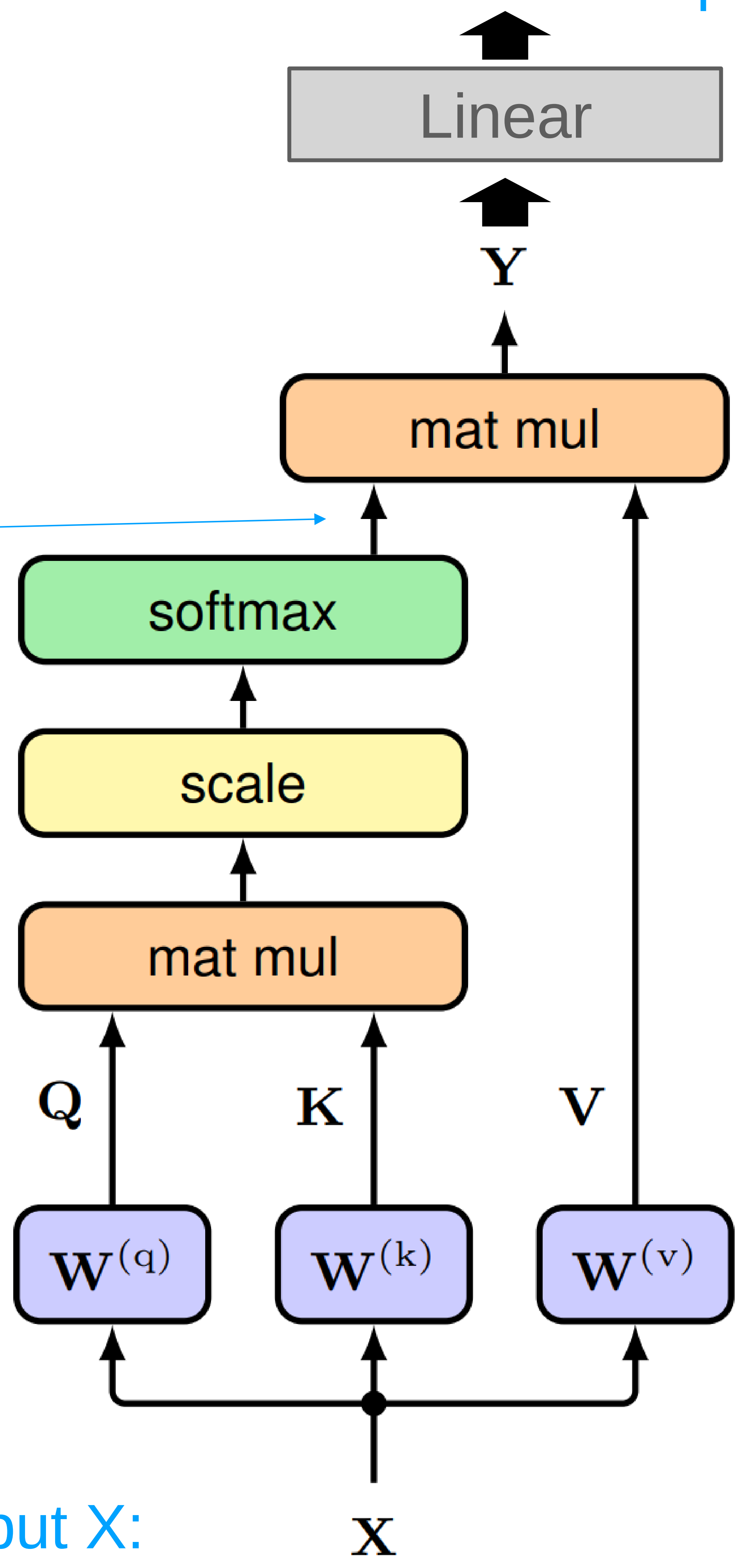
MHA (v0): information flow

Output: shape=[seq_len, d]

Add one more Linear layer for good measure.
Note: this Linear transform is done on each token independently, eg the Linear.W.shape is [d, d], NOT [seq_len, d]

Attention scores:
[seq_len, seq_len]

V: shape=[seq_len, d]



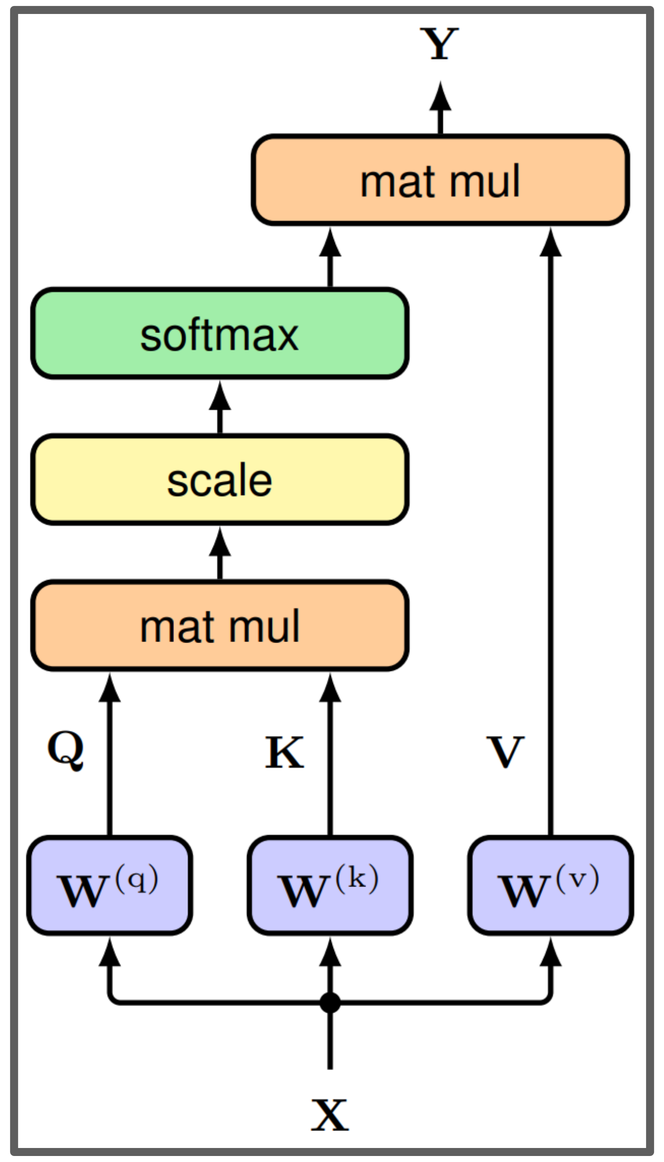
Q, K, V:
shape=[seq_len, d]

Input X:
shape=[seq_len, d]

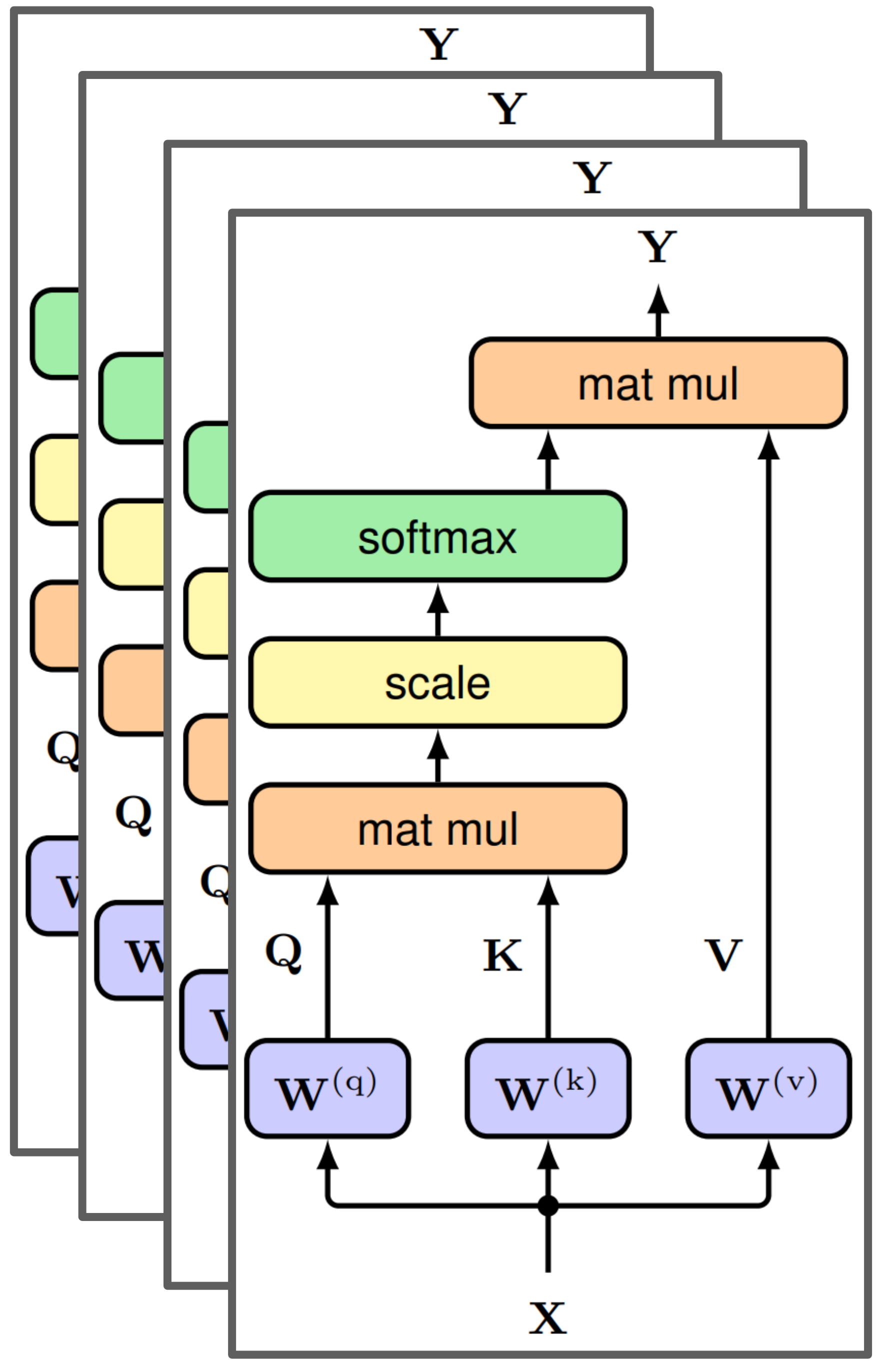
Intuition: use Q, K to compute attention scores. Then, transform X via V and the attention scores.

MHA (v1): multiple heads

- Idea: let's learn multiple self-attention modules (prev slide) in parallel at a given level (eg "width" of network)



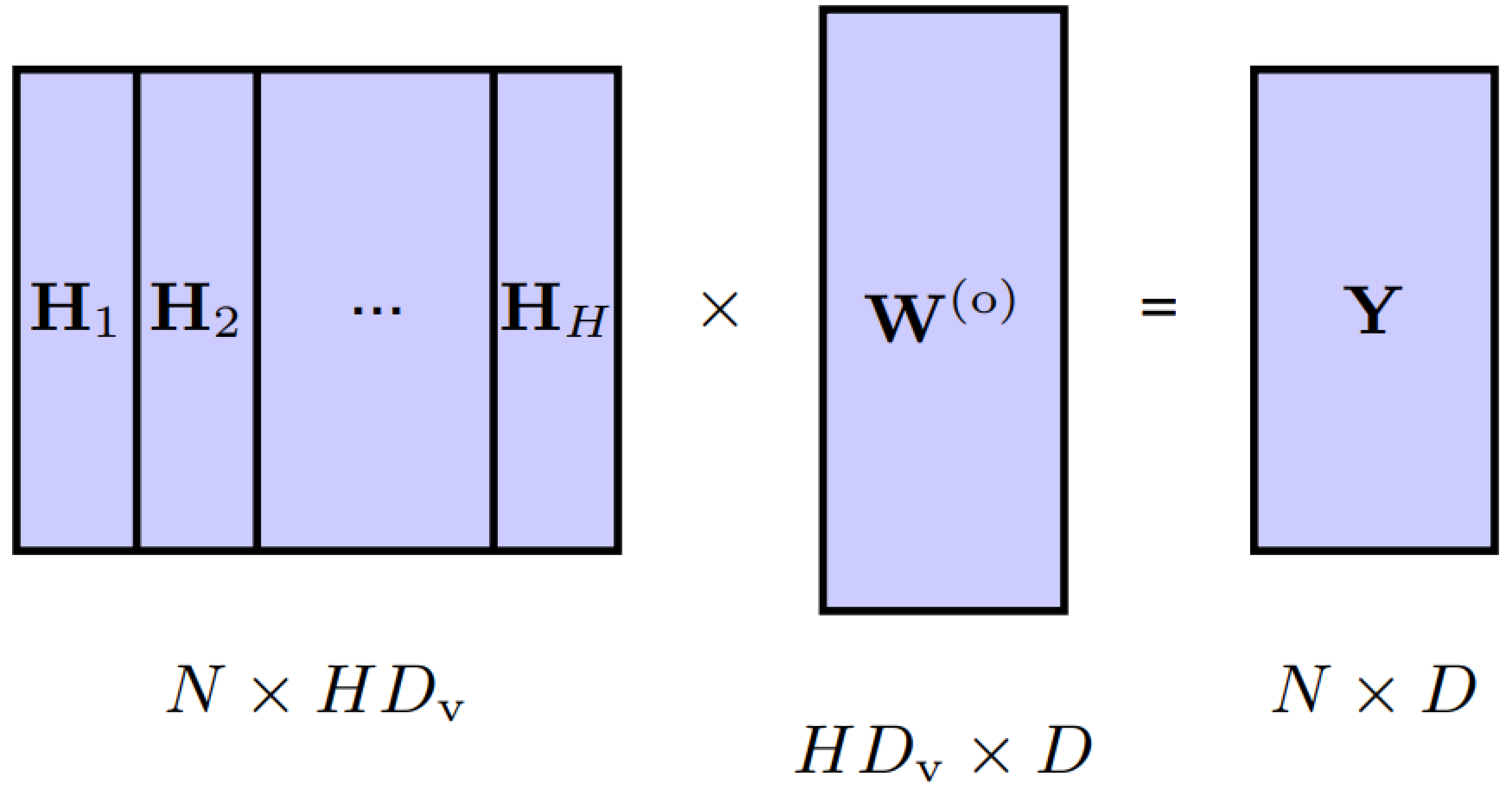
"single head"
attention



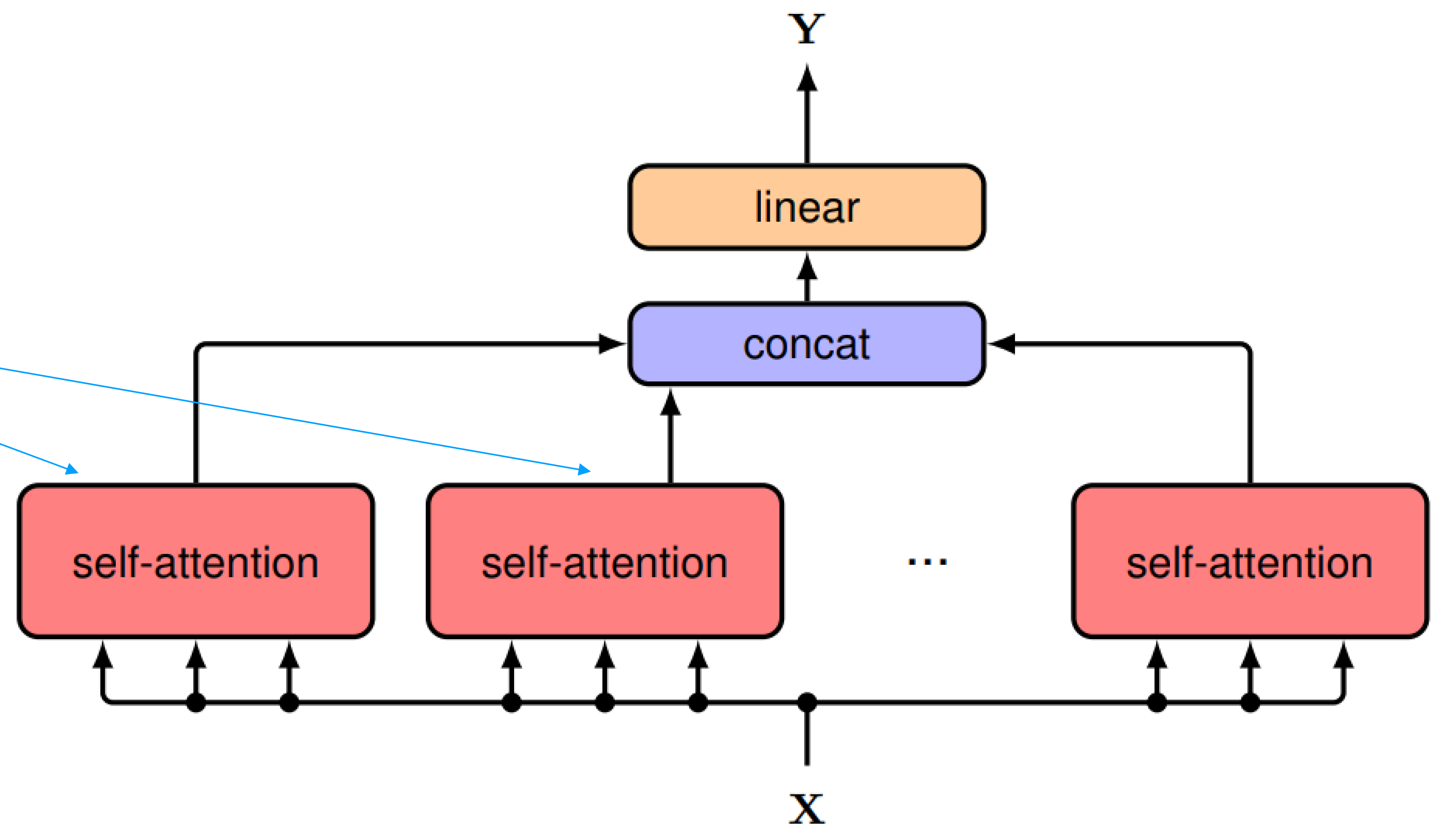
"multi head"
attention

MHA (v1): multiple heads

Let `h` be the number of heads.
(1) Run h different independent self-attention blocks, to produce h different outputs with shape=[seq_len, d]
(2) **Concatenate** all h outputs, and apply a learned linear transformation to produce the MHA output (shape=[seq_len, d])



$$\left.\begin{aligned}
\mathbf{Q}_h &= \mathbf{X}\mathbf{W}_h^{(q)} \\
\mathbf{K}_h &= \mathbf{X}\mathbf{W}_h^{(k)} \\
\mathbf{V}_h &= \mathbf{X}\mathbf{W}_h^{(v)} \\
\\
\mathbf{H}_h &= \mathrm{Attention}(\mathbf{Q}_h, \mathbf{K}_h, \mathbf{V}_h)
\end{aligned}\right\} \text{h different Q, K, V, and attention scores!}$$



$$\mathbf{Y}(\mathbf{X}) = \underbrace{\mathrm{Concat}\left[\mathbf{H}_1, \ldots, \mathbf{H}_H\right]}_{\text{shape=[seq\_len, h*d]}} \mathbf{W}^{(o)}$$

Learned linear transform. Shape=[h*d, d]

Nice property: we can easily stack MHA vertically ("deeper")!

Orig paper uses 6 layers, with h=8 heads

Neat animation from: https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

MHA (v1.5): multiple heads + split

In practice: to reduce computation costs, rather than have each self-attention module operate on the full embedding `d`, we **divide up the embeddings into `h` chunks.**

Example: for d=16 and h=2 heads,
Head0: work on first 8 embed dims: X[:, :8]
Head1: work on last 8 embed dims: X[:, 8:]

$$\mathbf{Q}_h = \mathbf{X}_h \mathbf{W}_h^{(q)}$$
$$\mathbf{K}_h = \mathbf{X}_h \mathbf{W}_h^{(k)}$$
$$\mathbf{V}_h = \mathbf{X}_h \mathbf{W}_h^{(v)}$$

X_h shape=[seq_len, d_h]

Q_h, K_h, V_h
Shape=[seq_len, d_h]

W_h^q, W_h^k, V_h^v
Shape=[d_h, d_h]

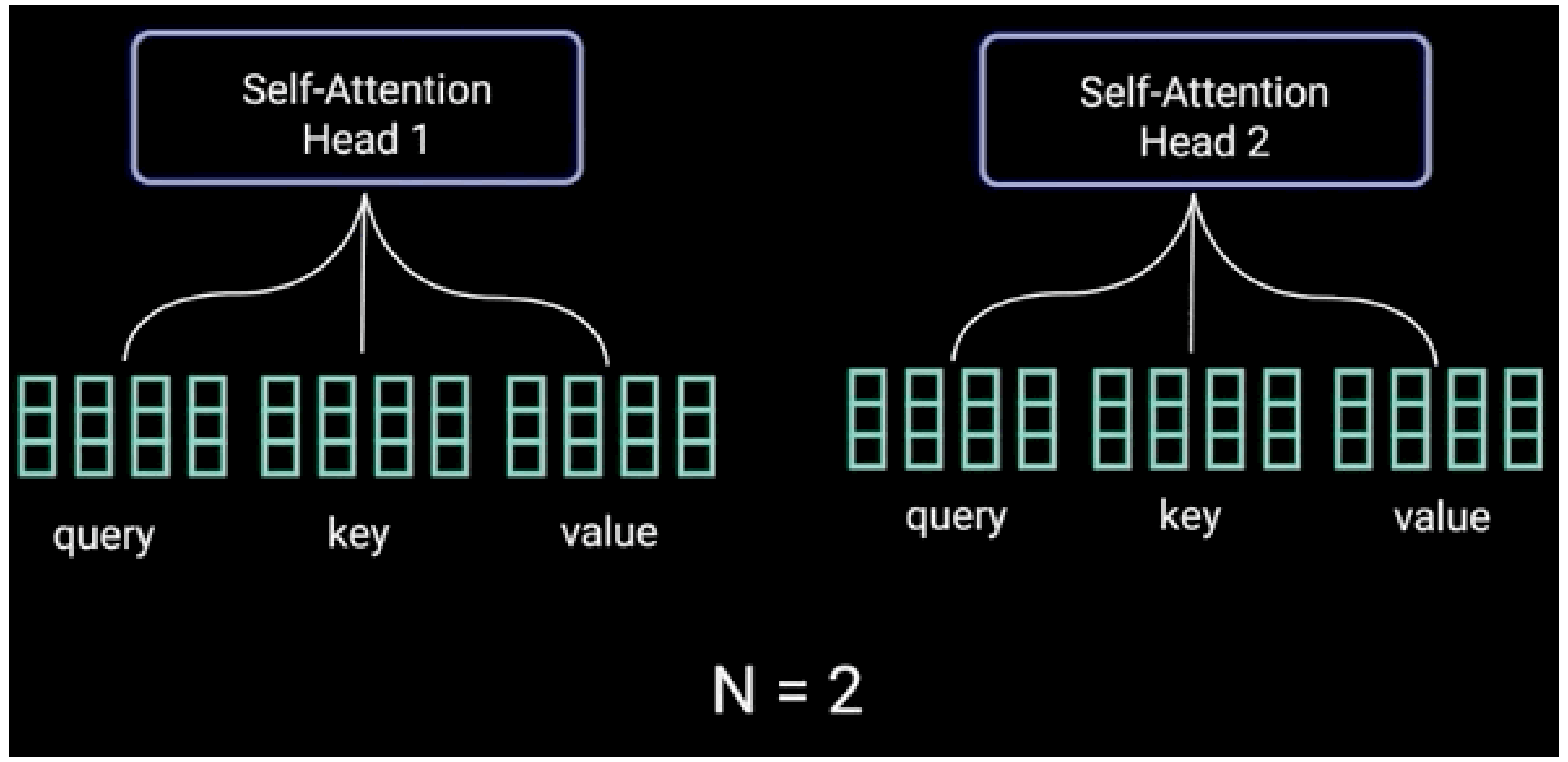
$$d_h = floor(\frac{d}{h})$$

"effective" embed dimensionality for each head

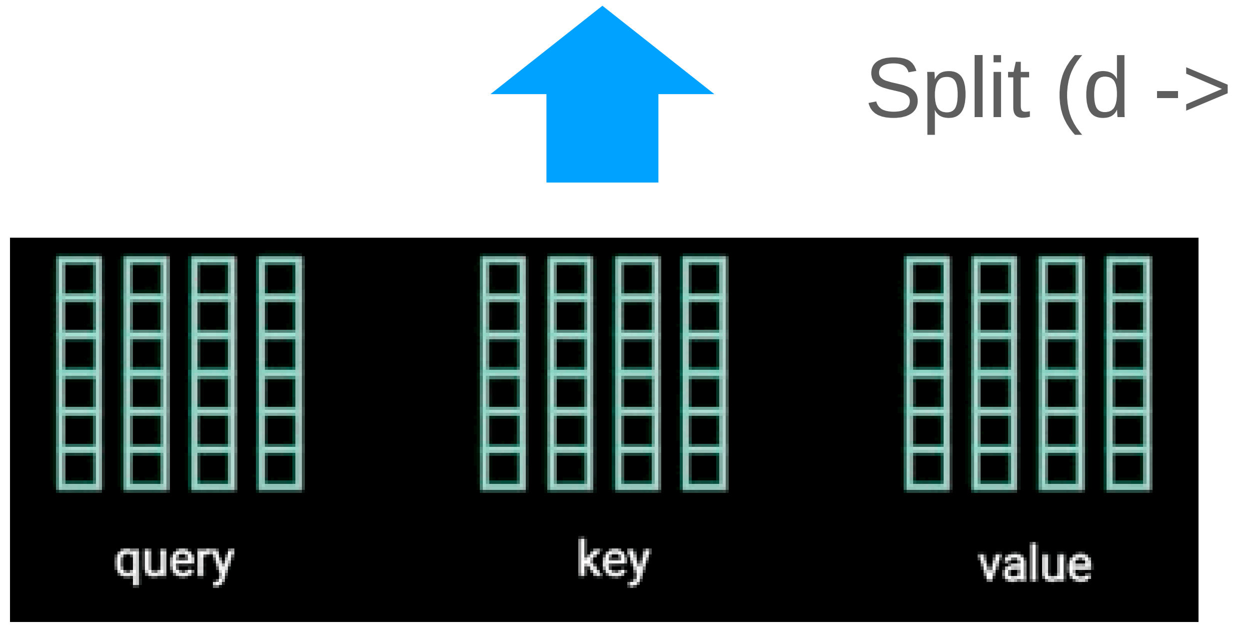
$$\mathbf{H}_h = \text{Attention}(\mathbf{Q}_h, \mathbf{K}_h, \mathbf{V}_h)$$

$$\mathbf{Y}(\mathbf{X}) = \underbrace{\text{Concat}\left[\mathbf{H}_1, \ldots, \mathbf{H}_H\right]}_{\text{shape=[seq\_len, } h*d_h\text{] =[seq\_len, d]}} \mathbf{W}^{(o)}$$

Learned linear transform. Shape=[d, d]



Splitting Q, K, V, N times before applying self-attention



Split (d -> d_h)

Implication: with this embedding "splitting", a MHA with h heads (operating on d//h dims) is roughly the same computation cost as a MHA with 1 head but operating on the full embedding dimensionality.

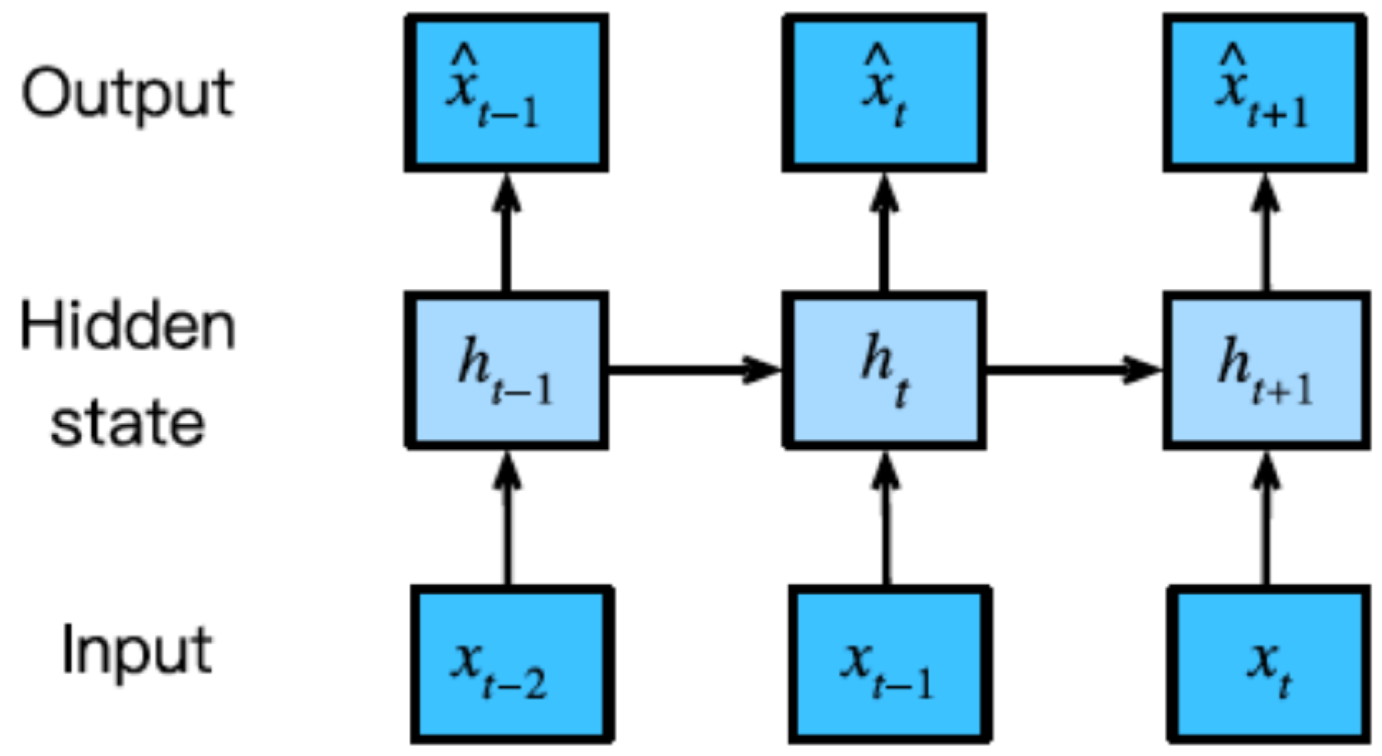
MHA: pytorch

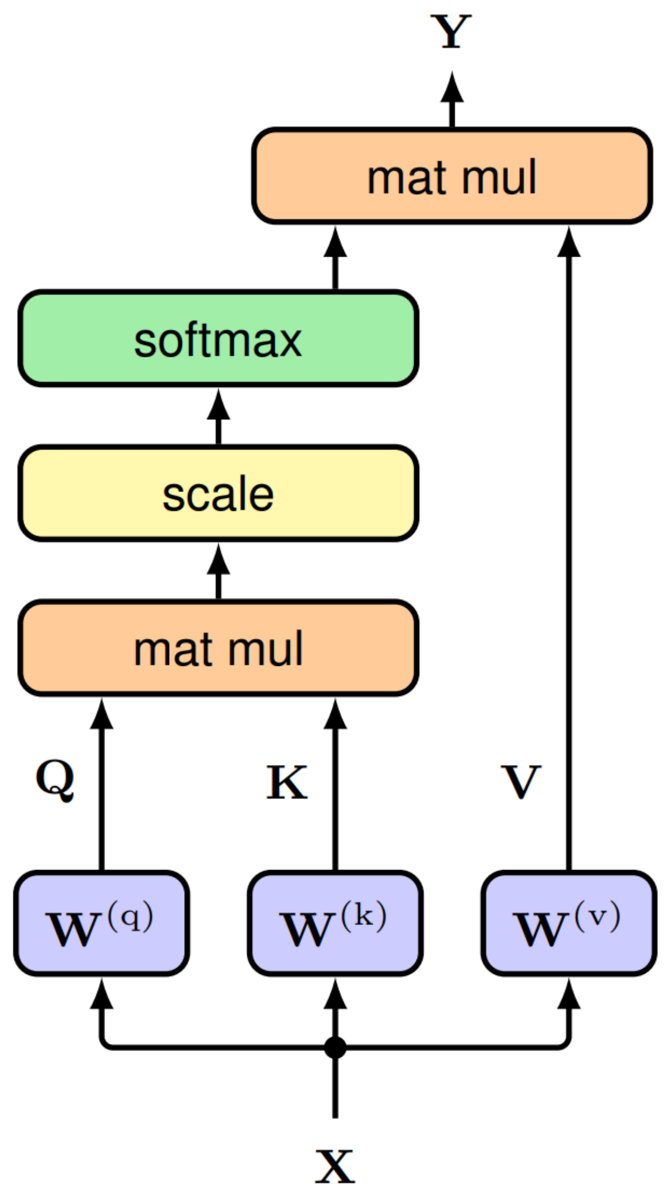
```python
import torch
input_seq_len = 8
batchsize = 2
embed_dim = 16
num_heads = 4
print(f"Scenario: input_seq_len={input_seq_len} batchsize={batchsize}
embed_dim={embed_dim} num_heads={num_heads}")

# https://pytorch.org/docs/stable/generated/torch.nn.MultiheadAttention.html
mha = torch.nn.MultiheadAttention(
    embed_dim=embed_dim,
    num_heads=num_heads,
    batch_first=True,
)

input_seq = torch.rand(size=[batchsize, input_seq_len, embed_dim],
dtype=torch.float32)
print(f"input_seq.shape: {input_seq.shape}")

out_mha, attn_weights = mha(query=input_seq, key=input_seq, value=input_seq,
need_weights=True)

print(f"out_mha.shape: {out_mha.shape}, attn_weights.shape:
{attn_weights.shape}")
out_proj_layer = mha.out_proj
print(f"out_proj_layer.weight.shape: {out_proj_layer.weight.shape}")
```

```
# Output
Scenario: input_seq_len=8 batchsize=2
embed_dim=16 num_heads=4
input_seq.shape: torch.Size([2, 8, 16])
out_mha.shape: torch.Size([2, 8, 16]),
attn_weights.shape: torch.Size([2, 8, 8])
out_proj_layer.weight.shape: torch.Size([16, 16])
```

Transformers: ordered sequences

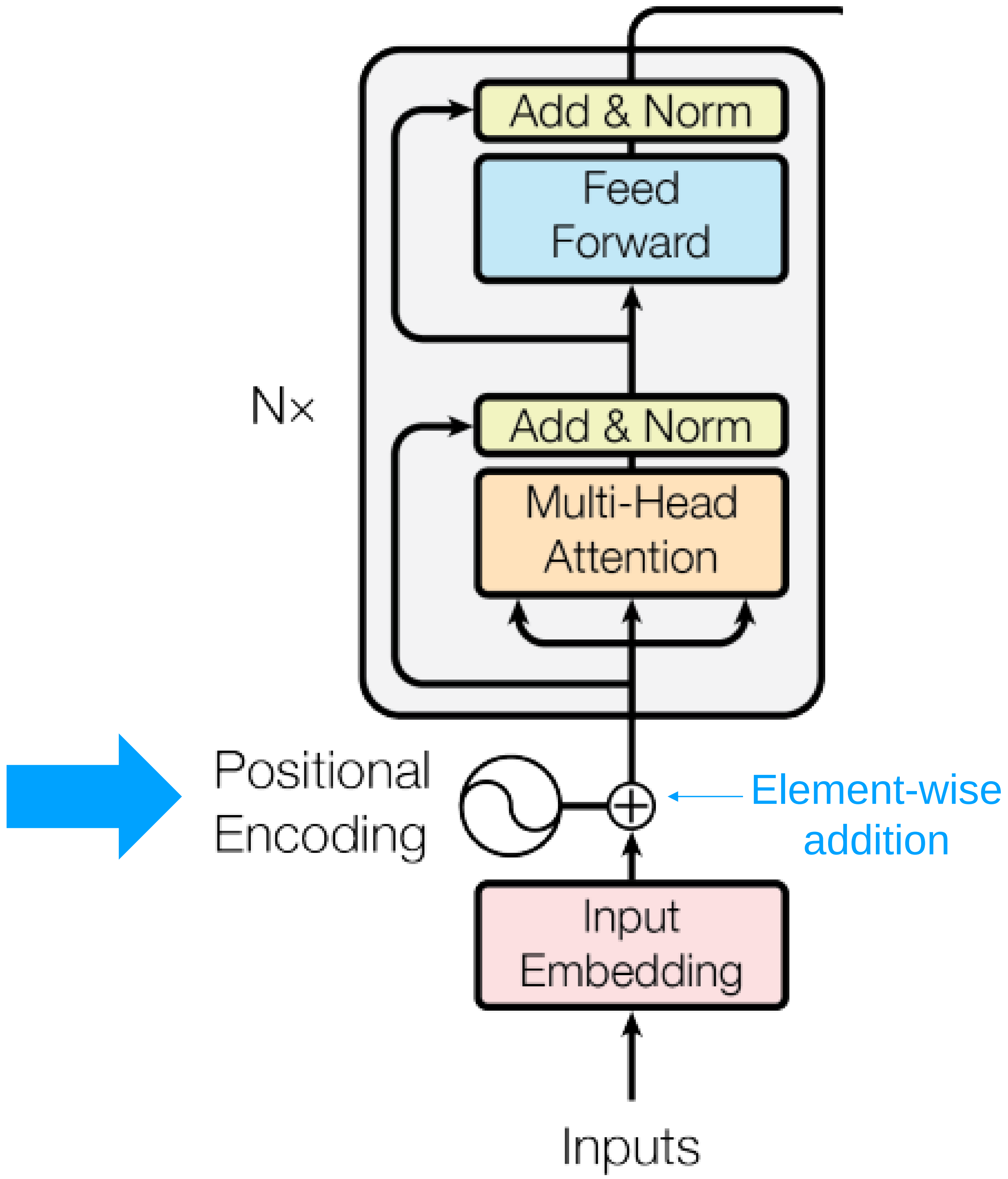
- Recall: in RNNs, we iteratively feed each input token to the model one at a time
  - Thus, token order information can be preserved, eg through the hidden state
- However: so far (as we've covered it), the MHA block ignores token ordering!
  - Ex: {"I", "am", "happy"} looks the same as {"am", "I", "happy"}.
    - Aka a "set" embedding, rather than a "sequence" embedding. Which is valuable in some scenarios, but not here.
  - When token order matters, this is concerning from a modeling standpoint...





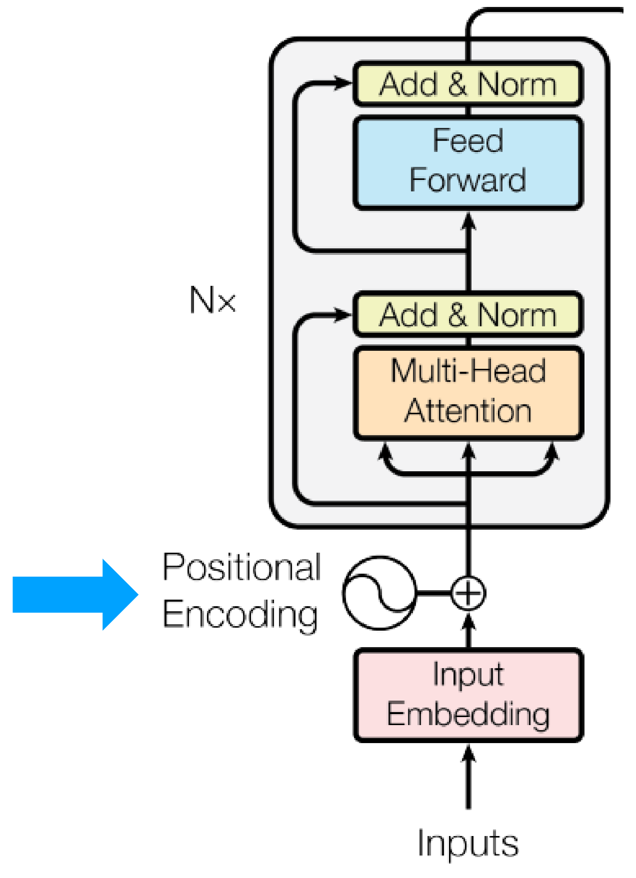
Positional encodings

- The transformers solution: **positional encodings**
- **Idea**: at the beginning of the transformer model, element-wise add a positional embedding (with the same dimensionality as the input X) to each token embedding before the first MHA block
- **Requirement**: Positional embedding must encode the "token position"



Positional encodings

- Positional embedding can either be learned (eg a torch.nn.Embedding bank), or hardcoded in a "special way"
  - Orig. paper used a sin/cos formula as the positional embedding



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

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

Where:
pos: sequence index
i: embedding dim index

```
# Let X be input seq (shape=[seq_len, d])
X_with_pos = torch.zeros(X.shape)
X_with_pos[0, 0] = sin(0 / (10000 ** (2*0 / d)))
X_with_pos[0, 1] = cos(0 / (10000 ** (2*1 / d)))
X_with_pos[0, 2] = sin(0 / (10000 ** (2*2 / d)))
...
X_with_pos[1, 0] = sin(1 / (10000 ** (2*0 / d)))
X_with_pos[1, 1] = cos(1 / (10000 ** (2*1 / d)))
X_with_pos[1, 2] = sin(1 / (10000 ** (2*2 / d)))
...
```

Alternate sin/cos along embed dim

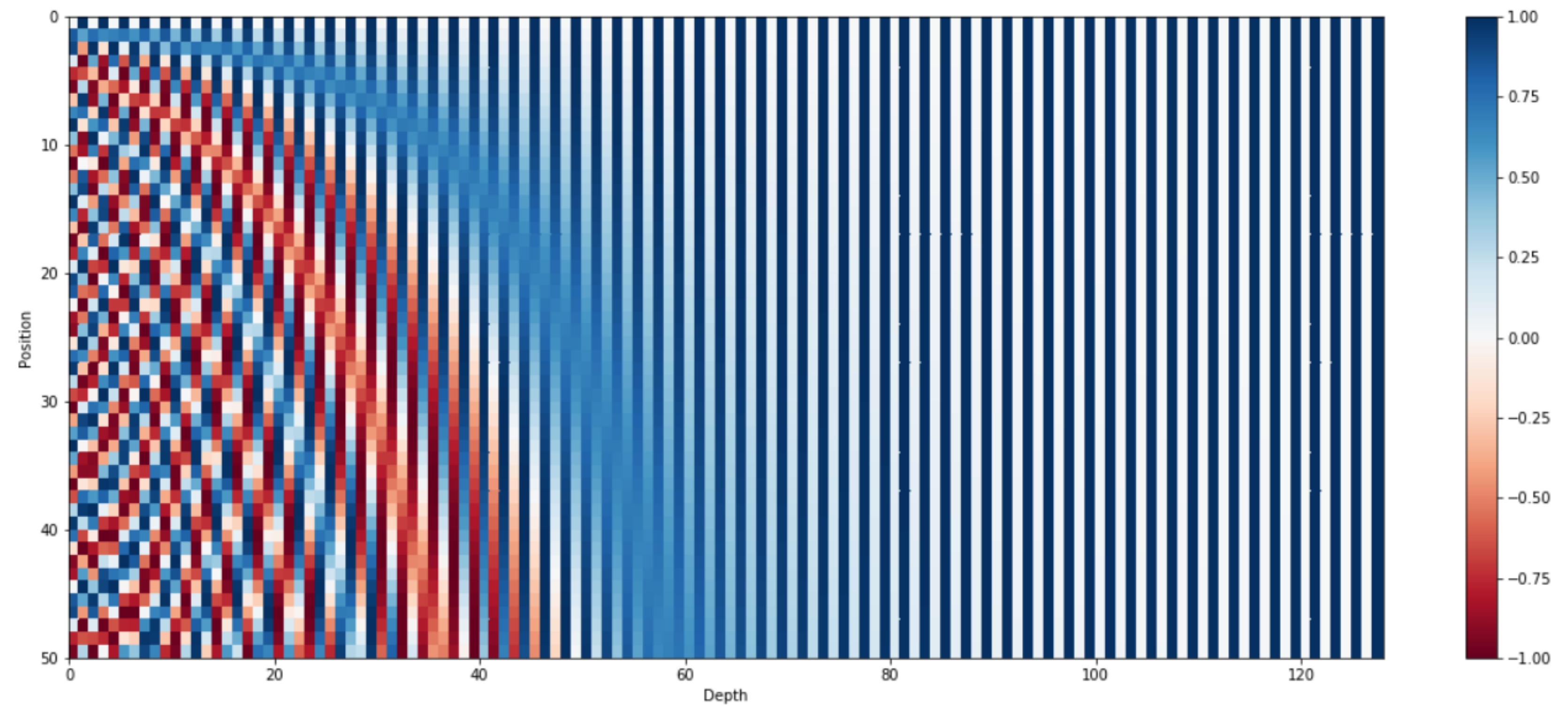


Figure 2 - The 128-dimensional positonal encoding for a sentence with the maximum lenght of 50. Each row represents the embedding vector $\vec{p_t}$

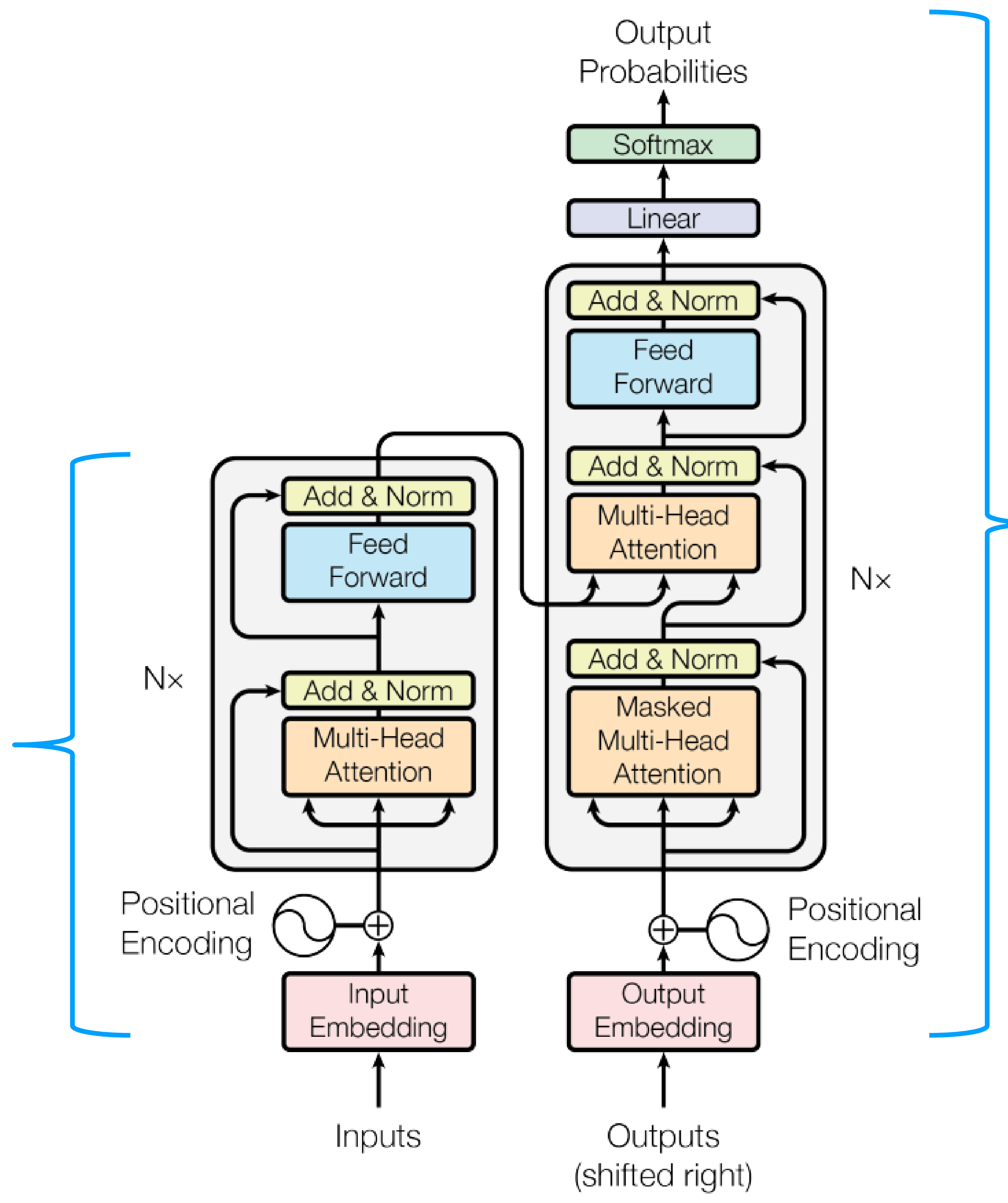
For more details/intuition on sin/cos, see: [link]

https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

Transformer: encoder and decoder

- The transformers paper originally discussed two components: an **Encoder**, and a **Decoder**
- **Encoder**: given an input sequence X, generate "good" token embeddings
- **Decoder**: given an input sequence X, generate output tokens Y
- First, let's focus on Encoders (it's conceptually simpler)

Encoder

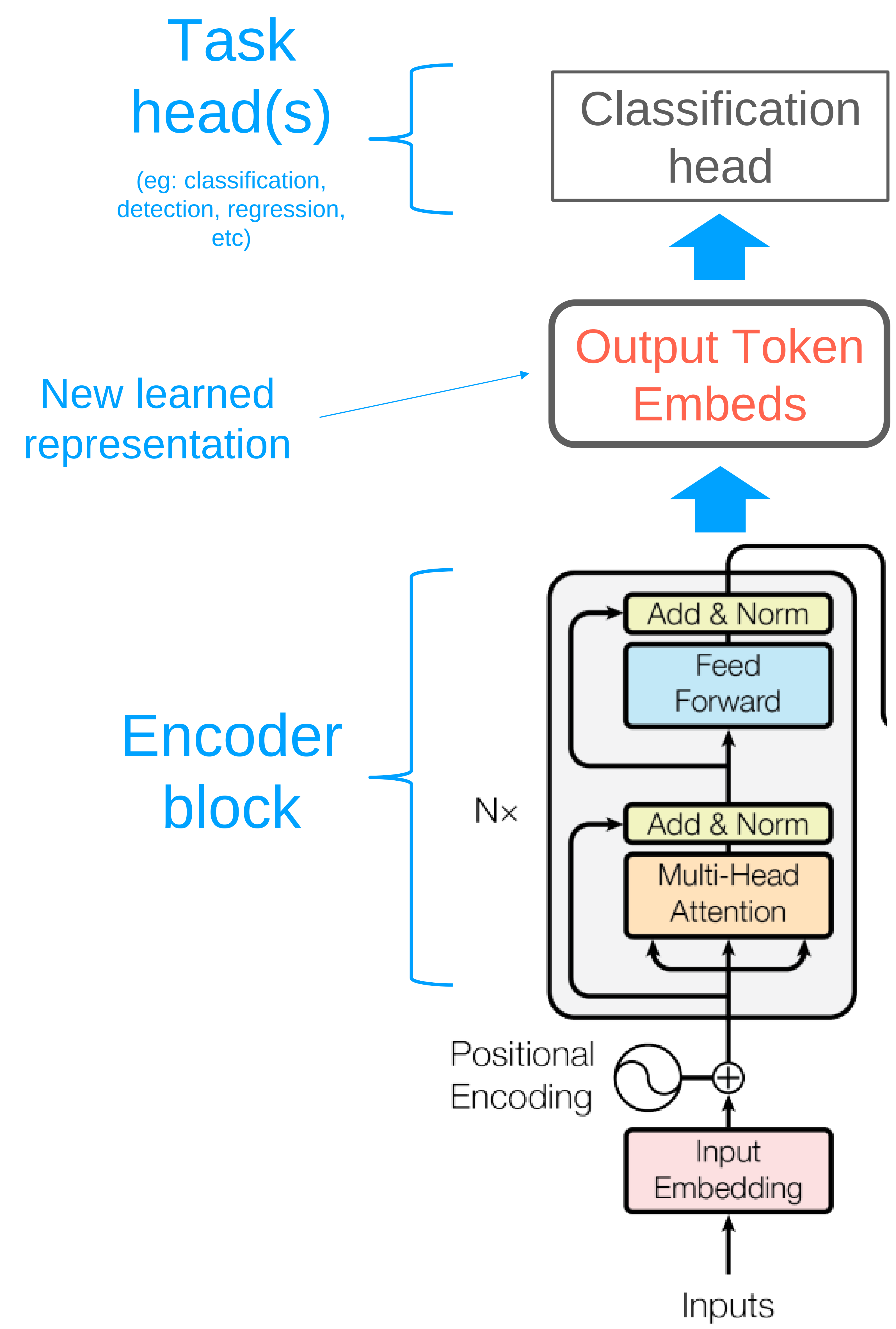


Decoder

Figure 1: The Transformer - model architecture.

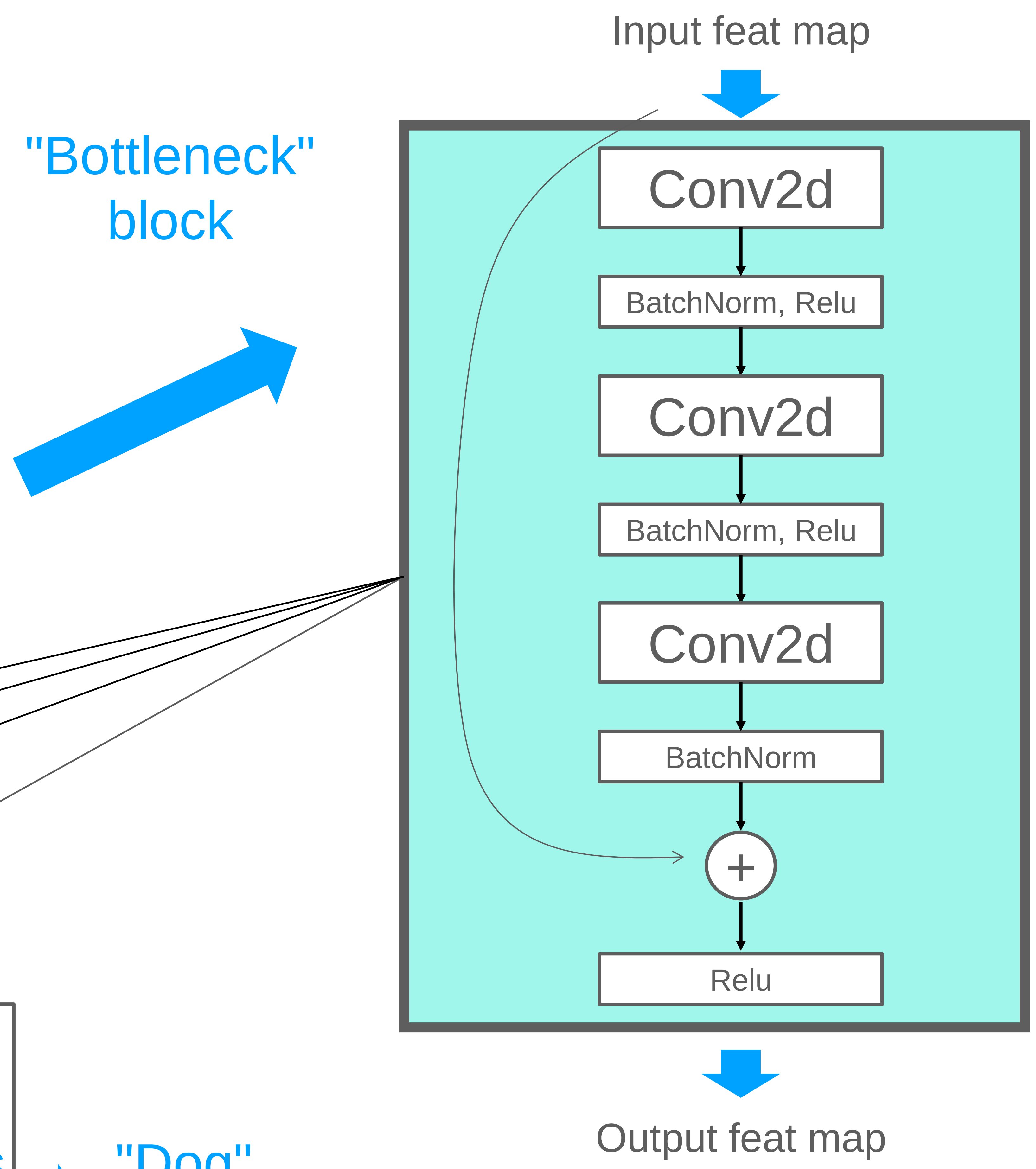
Encoder

- Input: X with shape=[bs, seq_len, dim]
- Output: X' with shape=[bs, seq_len, dim]
- **Idea**: learn a representation of the input sequence that is good for downstream tasks (eg classification, text generation, etc)

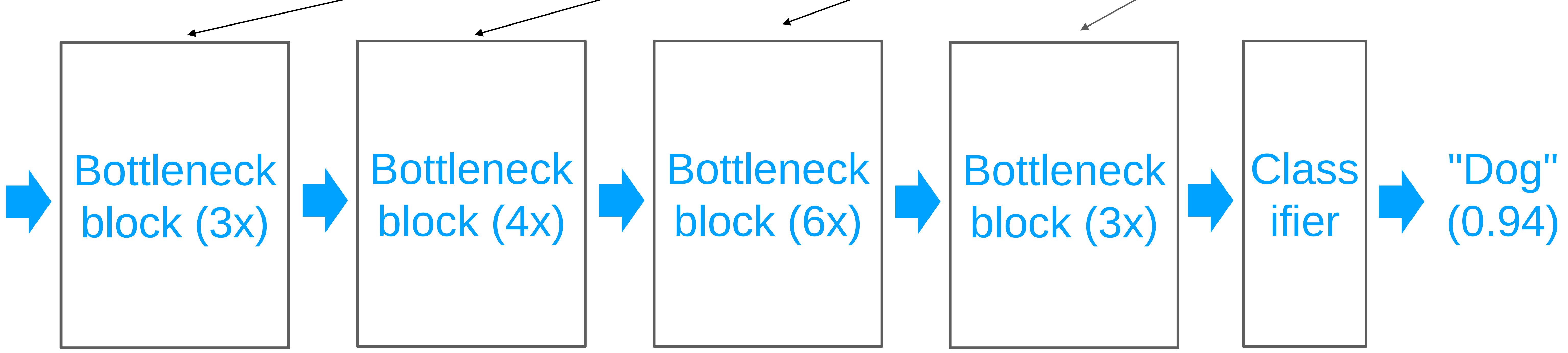


Aside: NN "blocks"

- It's common to define a DNN in terms of "blocks", rather than individual layers
  - Ex: a "ResNet Bottleneck Block" [link] consists of:



ResNet50 (Image classification arch [link]) is then built by repeating the "Bottleneck block" a bunch of times

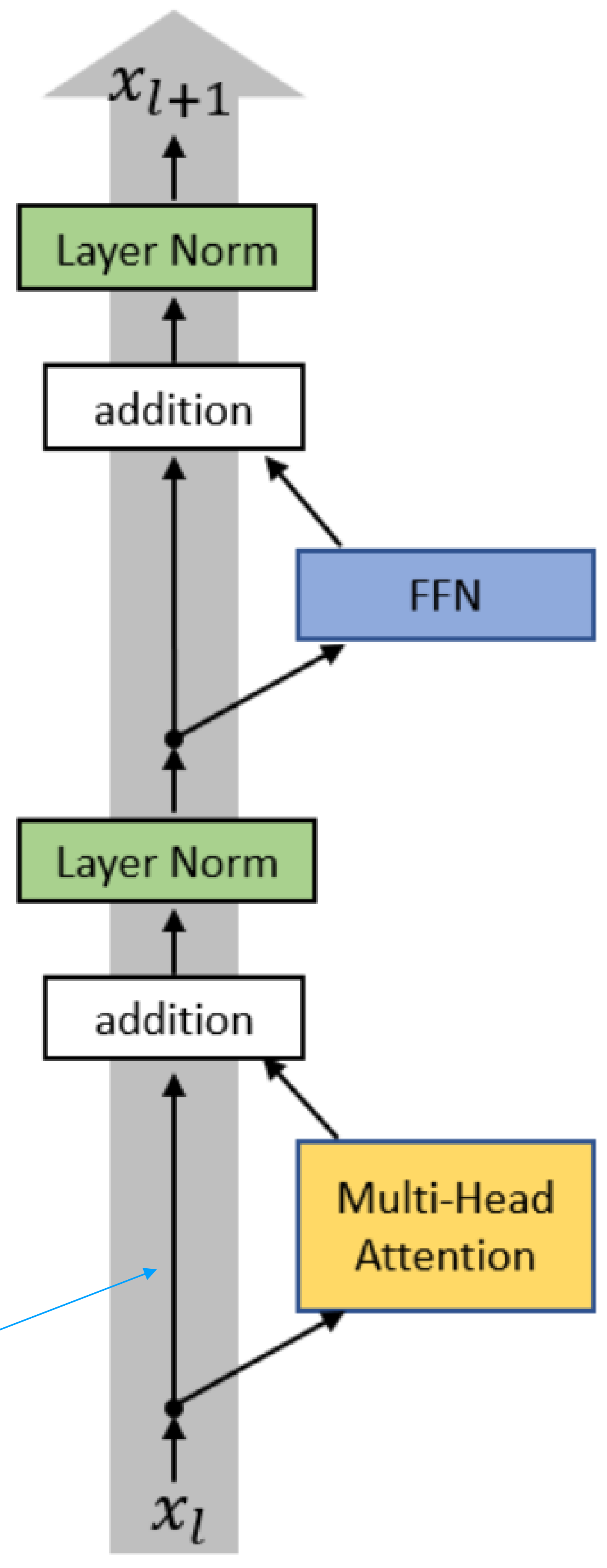


* Some things missing from this resnet50 picture: initial "stem", downsampling (spatial resolution) layers, other minor details

If you're curious here is pytorch's (torchvision) implementation of ResNet50 (in all of its gory detail): [link]
Tip: you should be able to read this code and understand 90% of what's going on! The implementation is complicated because it's super generic+flexible, but with some study you can see what's going on :)

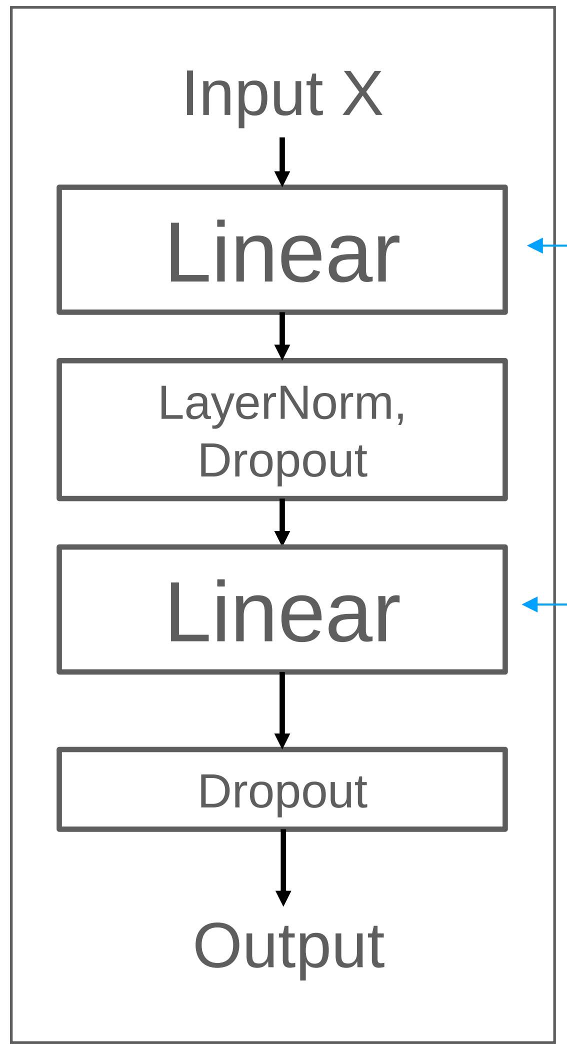
Encoder block

Source:
[TransformerEncoderLayer.forward()]



(a)

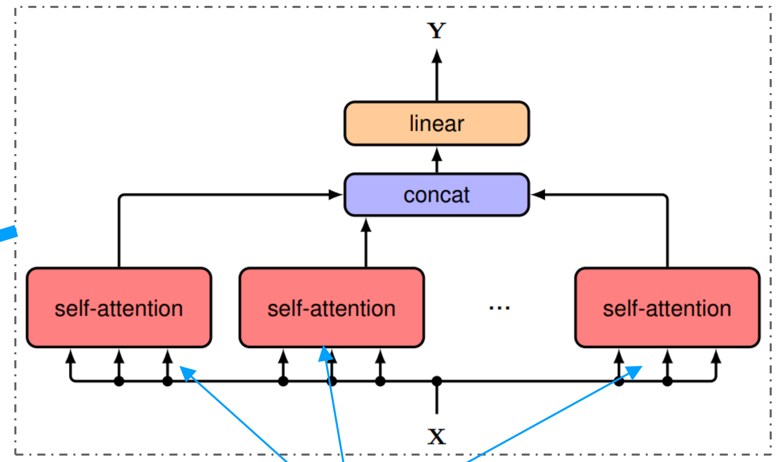
Residual/skip
connection

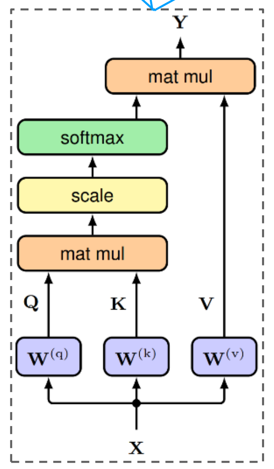


Linear(in=dim_embed,
out=dim_ff=2048)

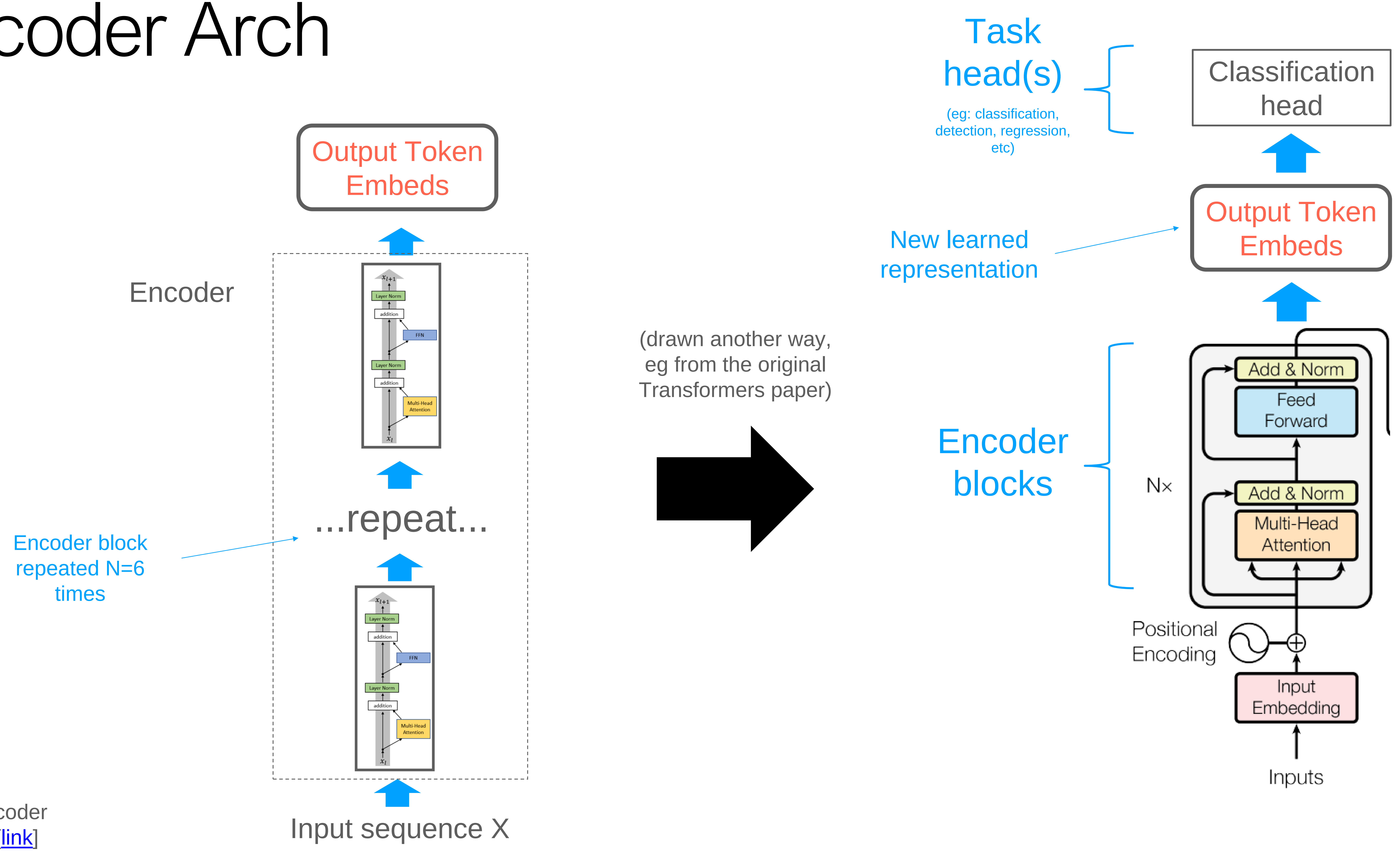
Linear(in=dim_ff=2048,
out=dim_embed)

Source:
[TransformerEncoderLayer._ff_block()]





Encoder Arch



TransformerEncoder pytorch code: [link]

Detail: Pre-norm vs Post-norm

- Original transformers paper did "Post-LayerNorm" (Post-LN)
- But, smart people found out that "Pre-LayerNorm" (Pre-LN) works better
  - Better training stability, can use larger learning rate, etc
  - For more details, see: [link]

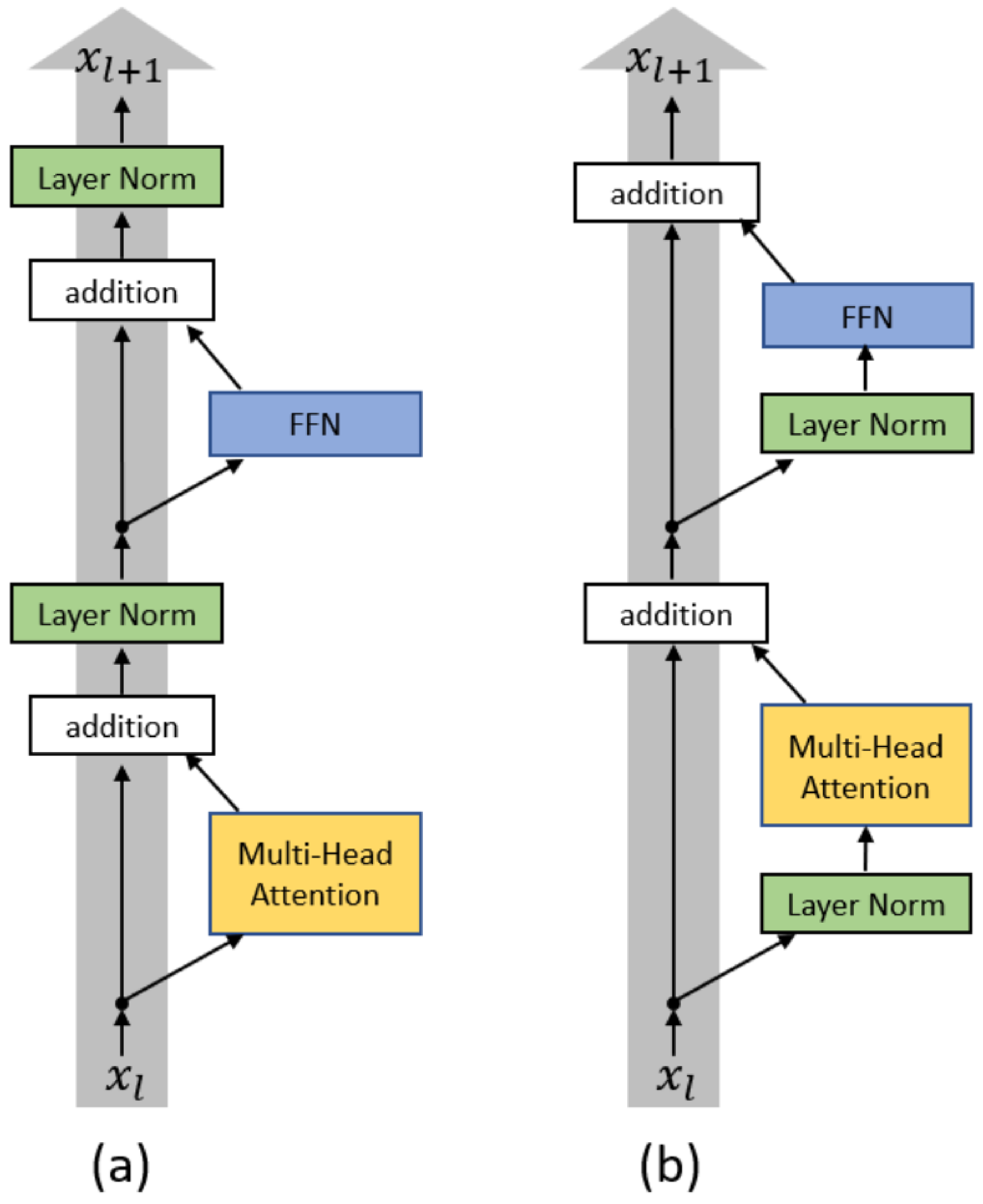
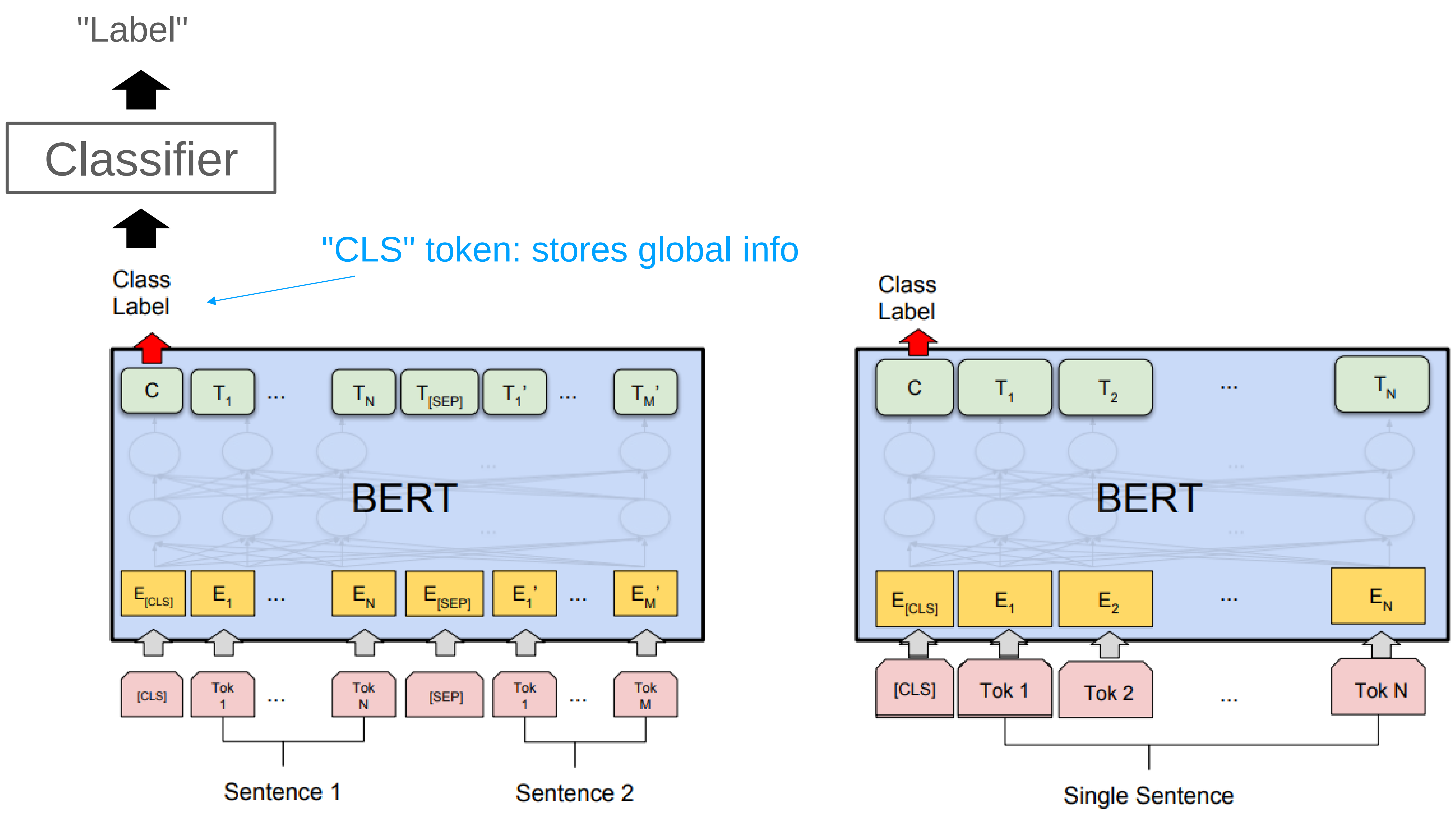


Figure 1. (a) Post-LN Transformer layer; (b) Pre-LN Transformer layer.

(Left) Original version. (Right) "Improved" version

Application: text classification (Bert)

- BERT ("Bidirectional Encoder Representations from Transformers"): [link]
- Perform text sentence classification using a Transformer Encoder + pretraining/finetuning
- Key idea: prepend a "**CLS**" token to the start of every sequence. Then, train a classifier on top of this CLS token embedding
  - Intuition: CLS token stores the "global" info about the sentence

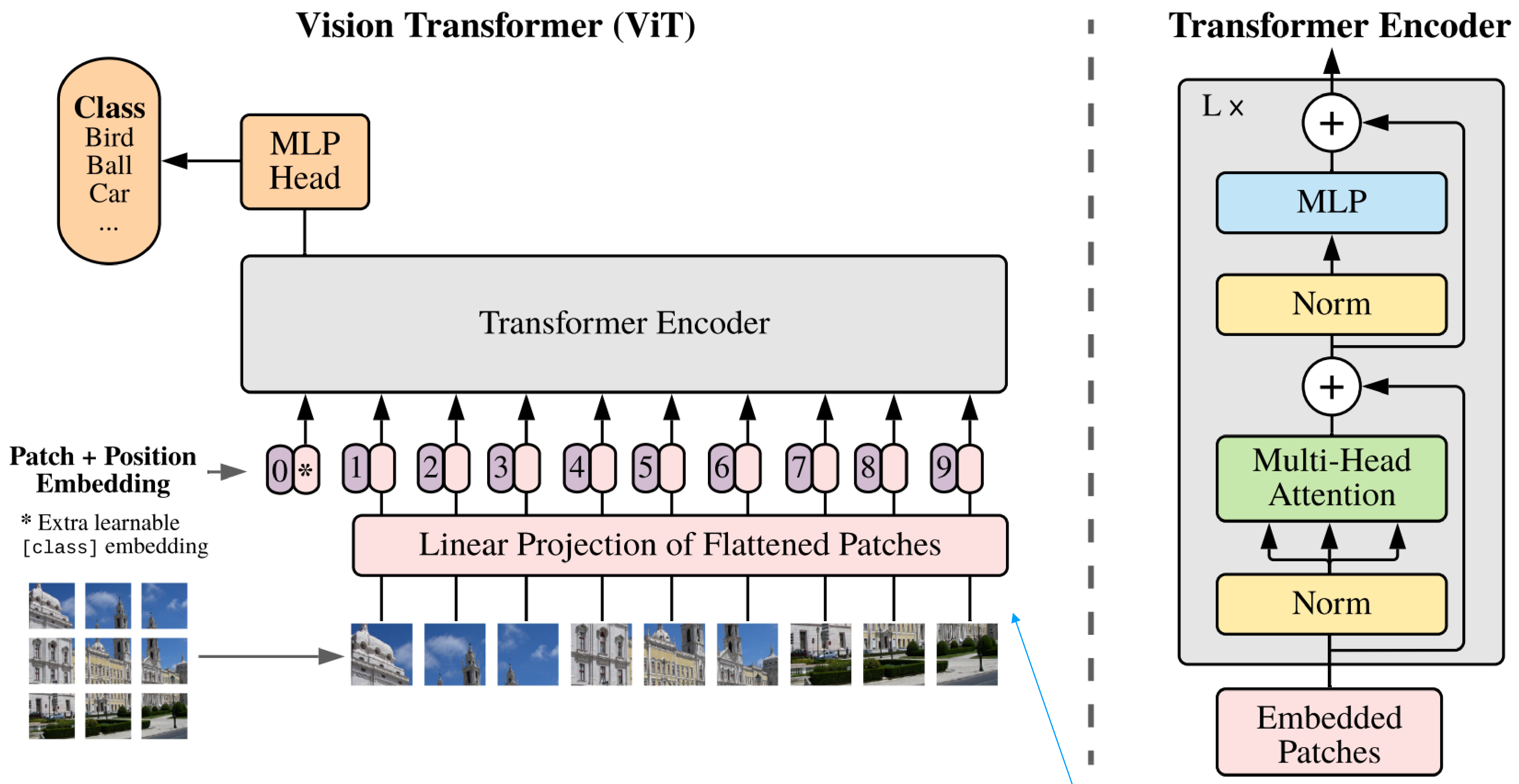


(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG

(b) Single Sentence Classification Tasks: SST-2, CoLA

Application: image classification (ViT)

- "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale" [link]
- Image classification with Transformer Encoder
- Idea: represent an image as a sequence of image patches!



Fun fact: this "linear projection of flattened patches" is basically a Conv2d, which people laughed about for awhile...