Self-Attention, Transformer, and Graph Networks

Xiaolong Wang

Previous classes

- RNN for time sequence processing

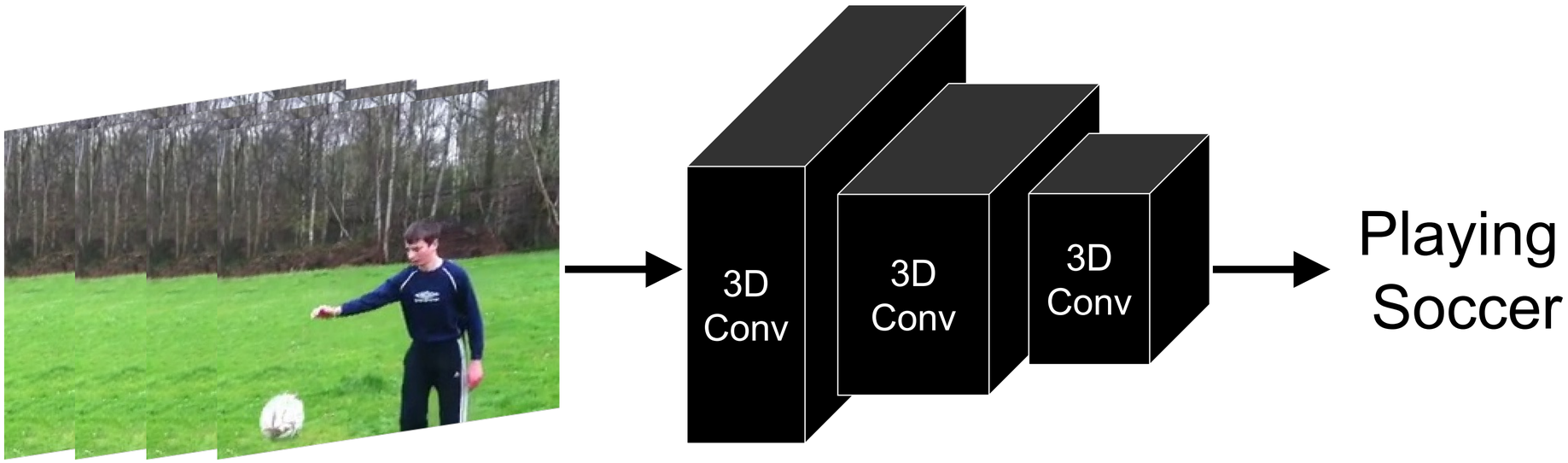
- Video understanding with temporal convolution, 3D CNN

This Class

- Non-local Neural Network for Videos
- Self-Attention and Transformer for NLP
- Graph Neural Networks

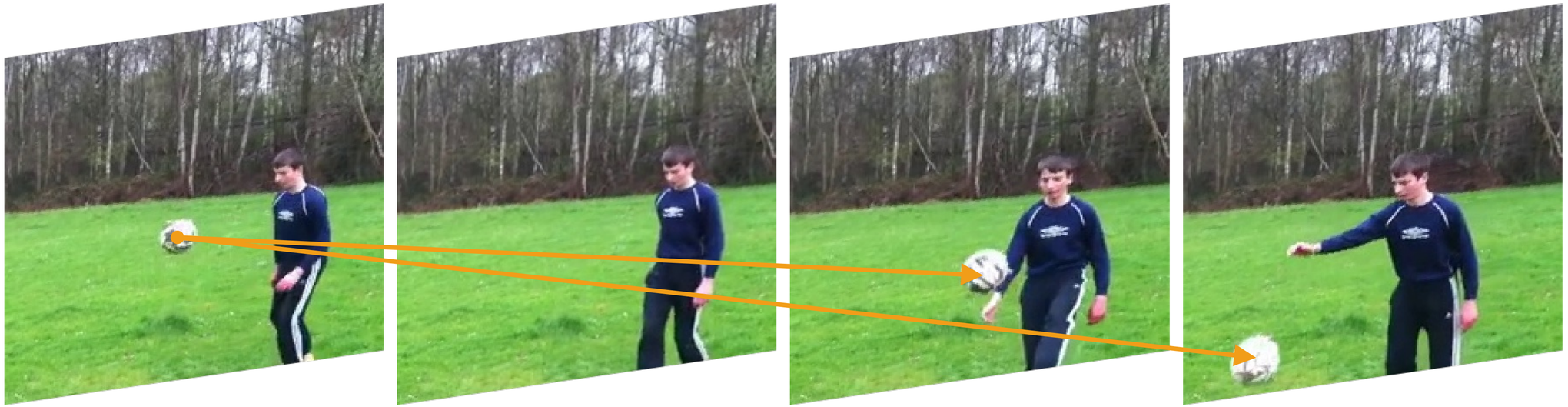
Non-local Neural Network for Videos

Video Recognition



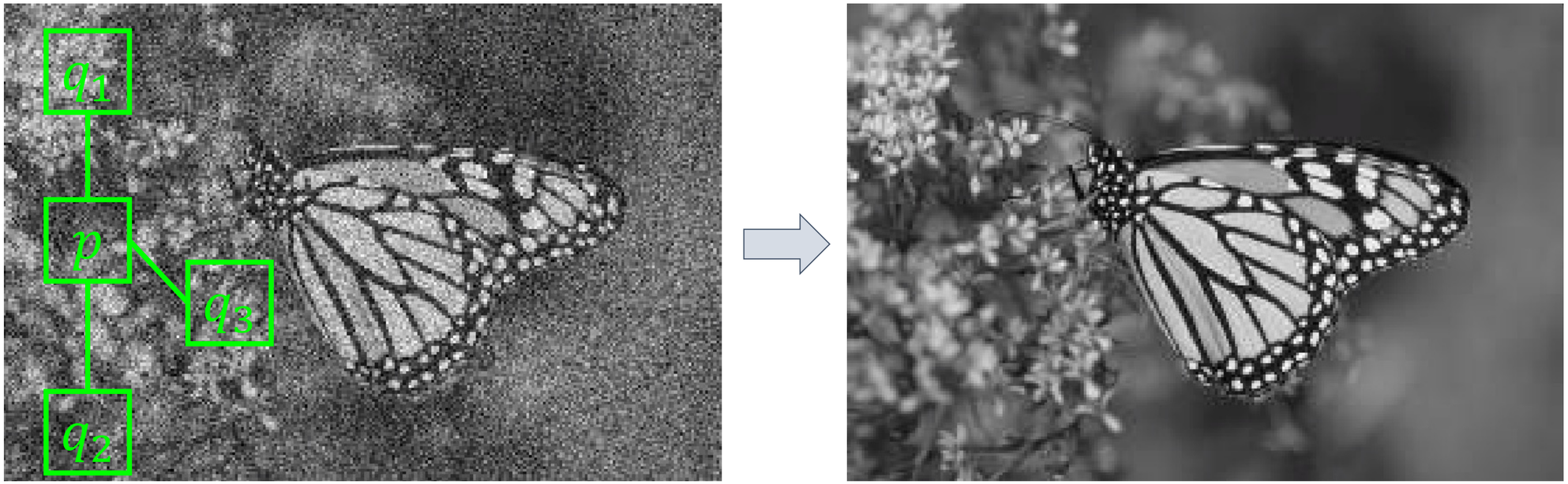
Reasoning for Action Recognition

Long-rang explicit reasoning



Wang et al., 2018.

Non-local Means

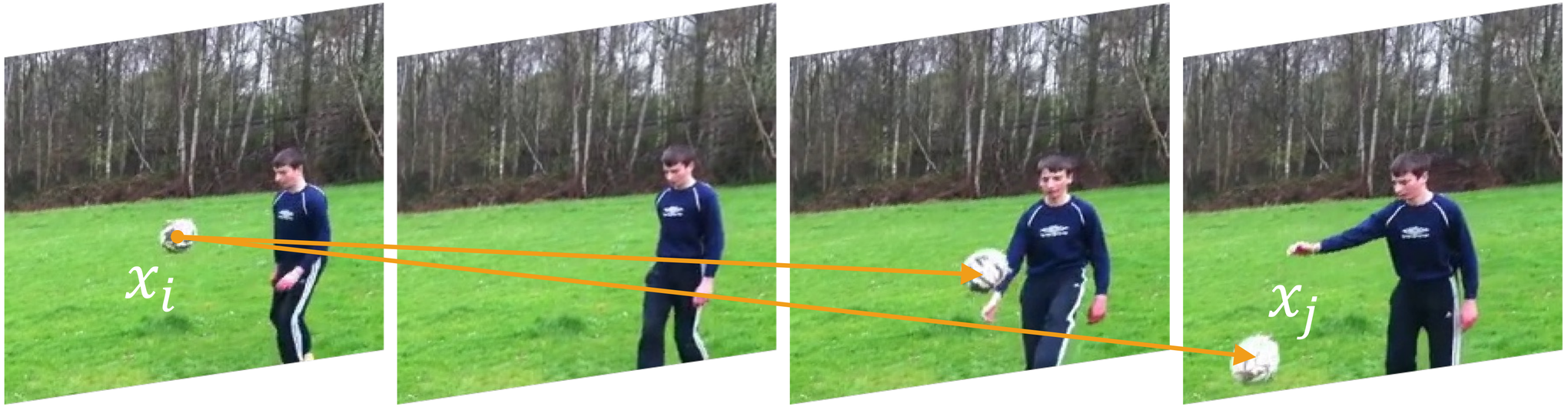


Buades et al., 2005.

Non-local Operator

Operation in feature space

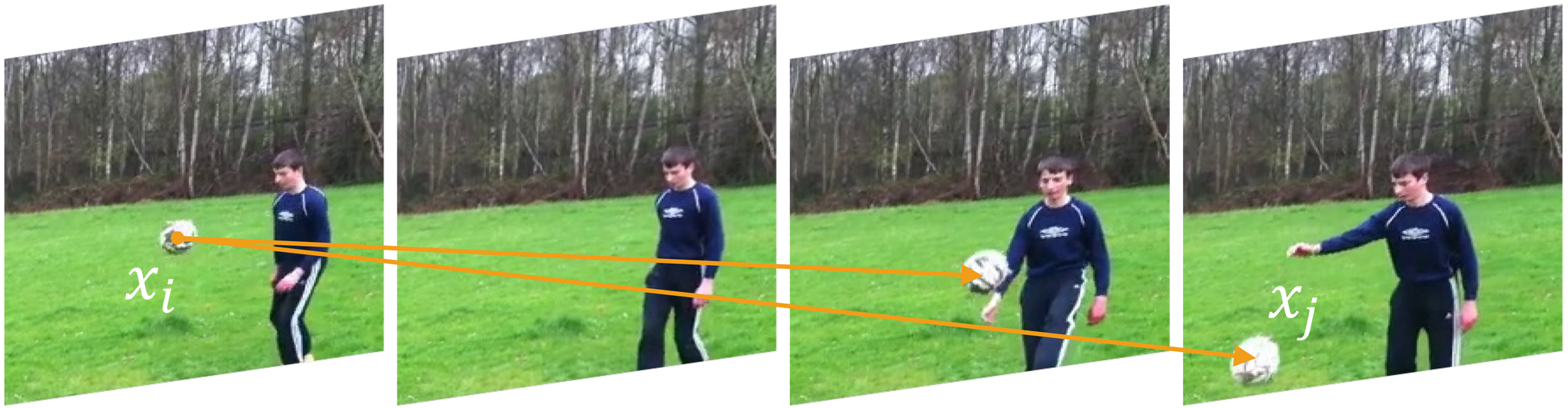
Can be embedded into any ConvNets



Non-local Operator

$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j) \; g(x_j)$$

Affinity Features



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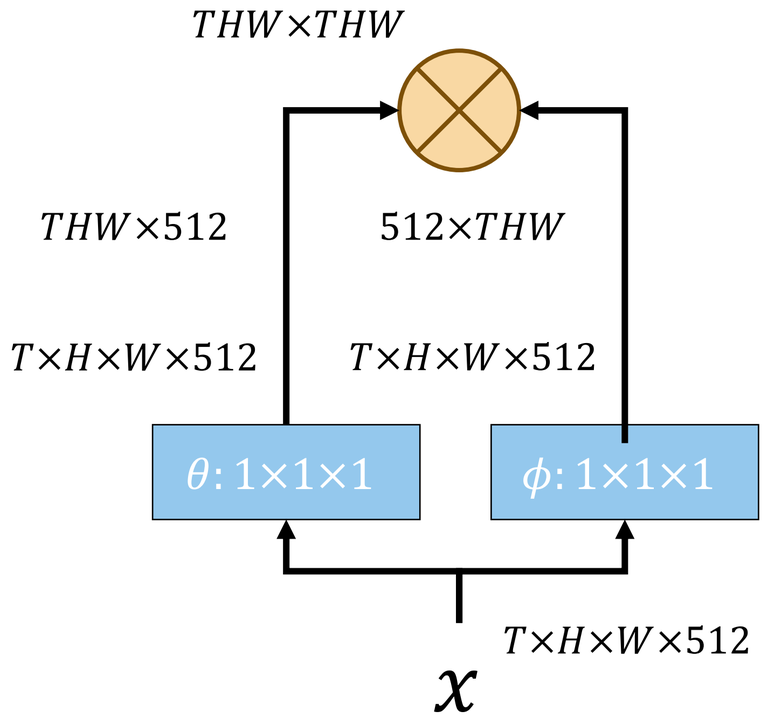

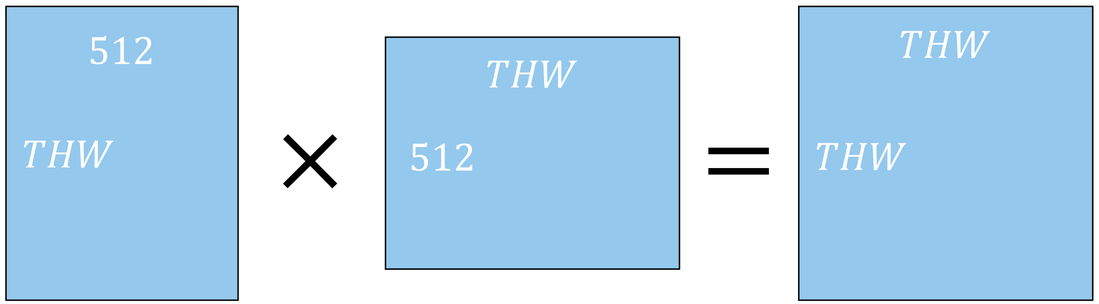

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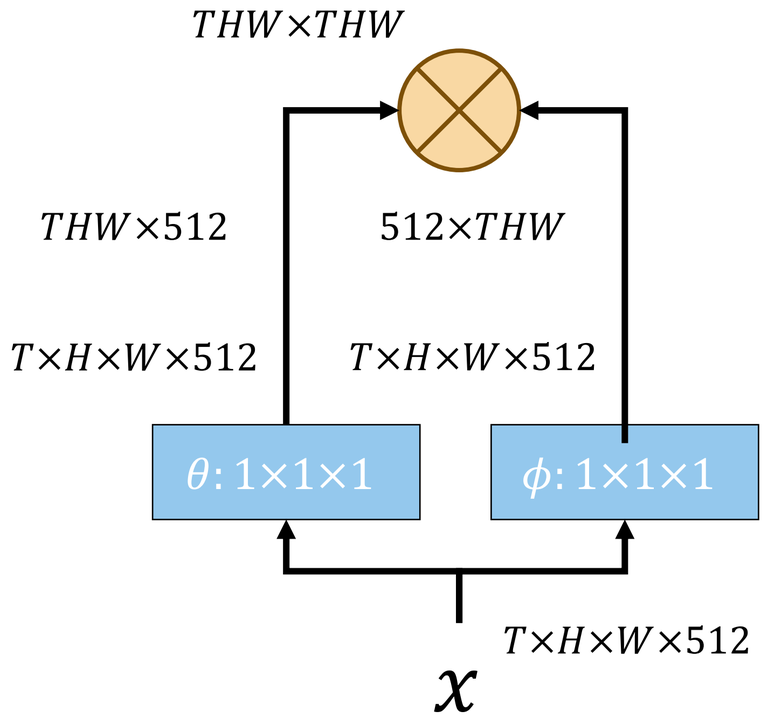

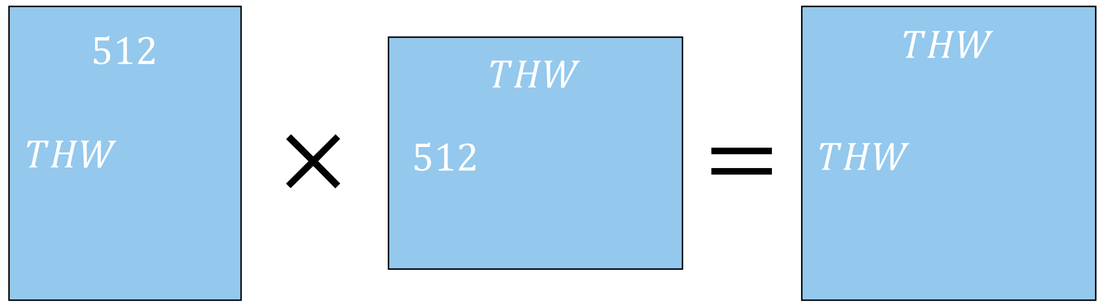

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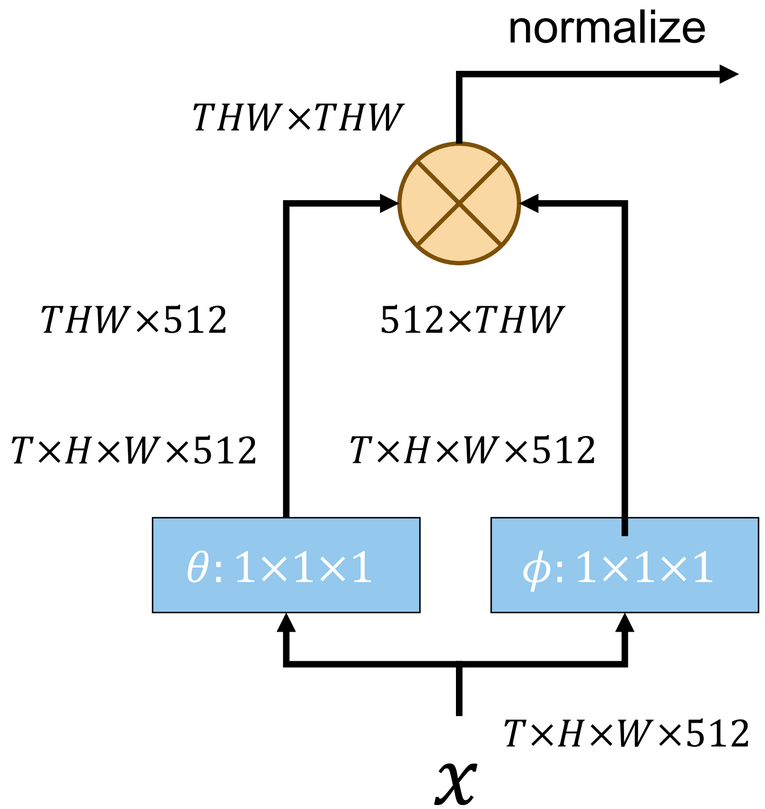
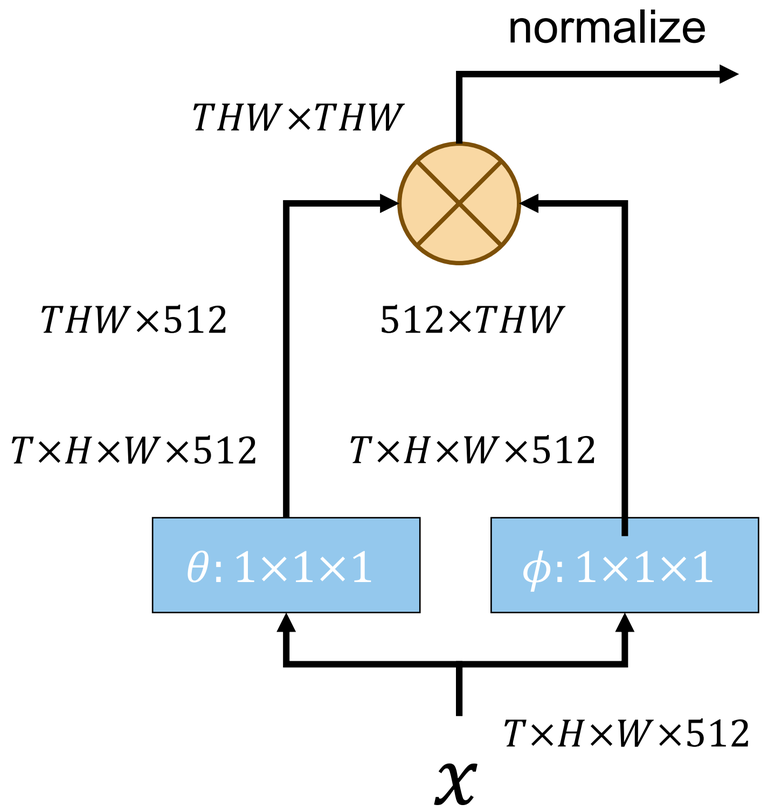


Non-local Operator

$$y_i = \frac{1}{C(x)} \sum_{\forall j} f\left(x_i, x_j\right)\ g(x_j)$$



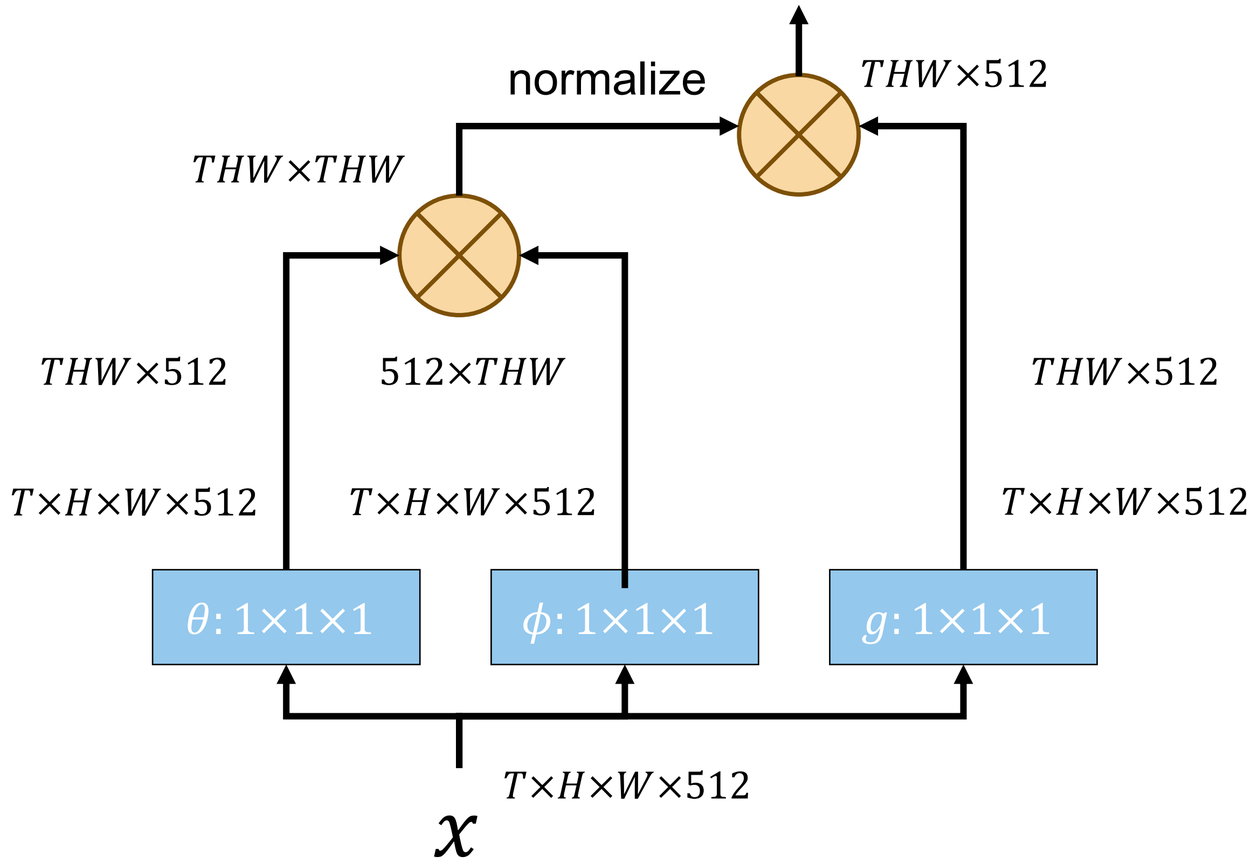
$$f\left(x_i, x_j\right) = \exp(x_i^T x_j)$$

$$C(x) = \sum_{\forall j} f\left(x_i, x_j\right)$$

$$\frac{f\left(x_i, x_j\right)}{C(x)} = \frac{\exp(x_i^T x_j)}{\sum_{\forall j} \exp(x_i^T x_j)}$$

Non-local Operator

$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$



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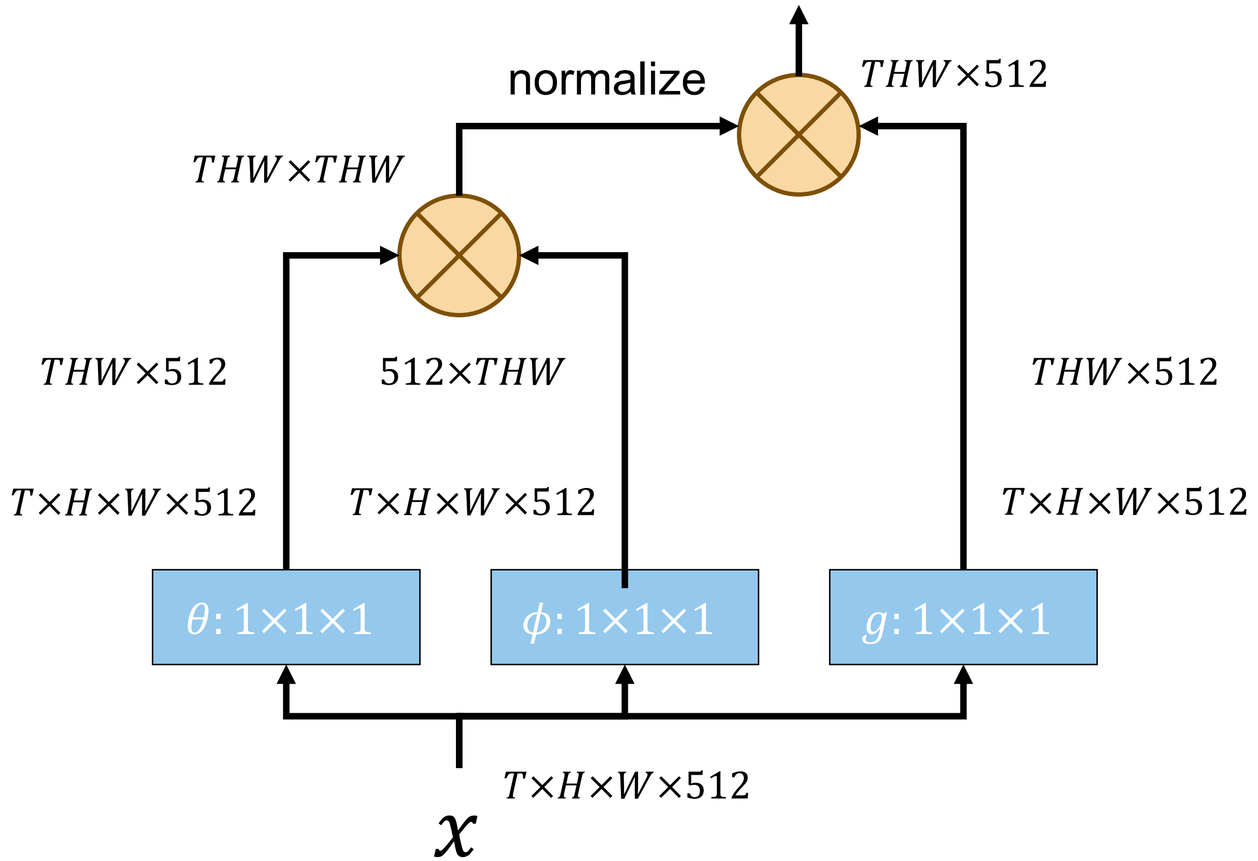
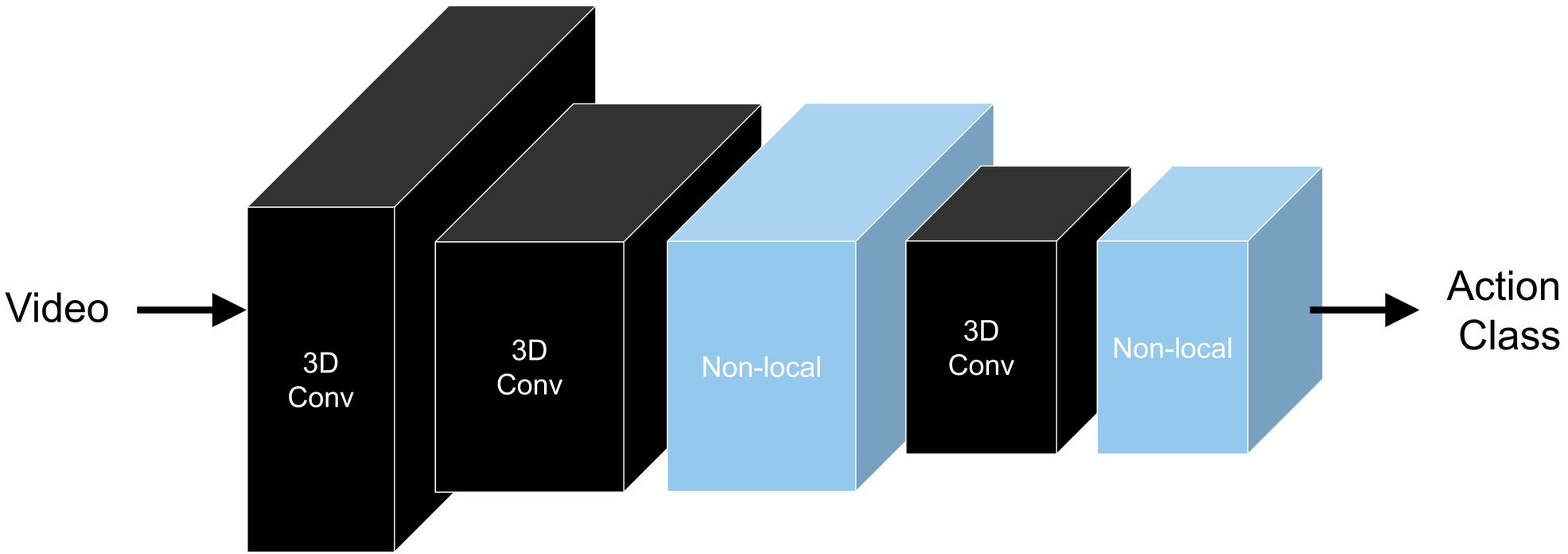
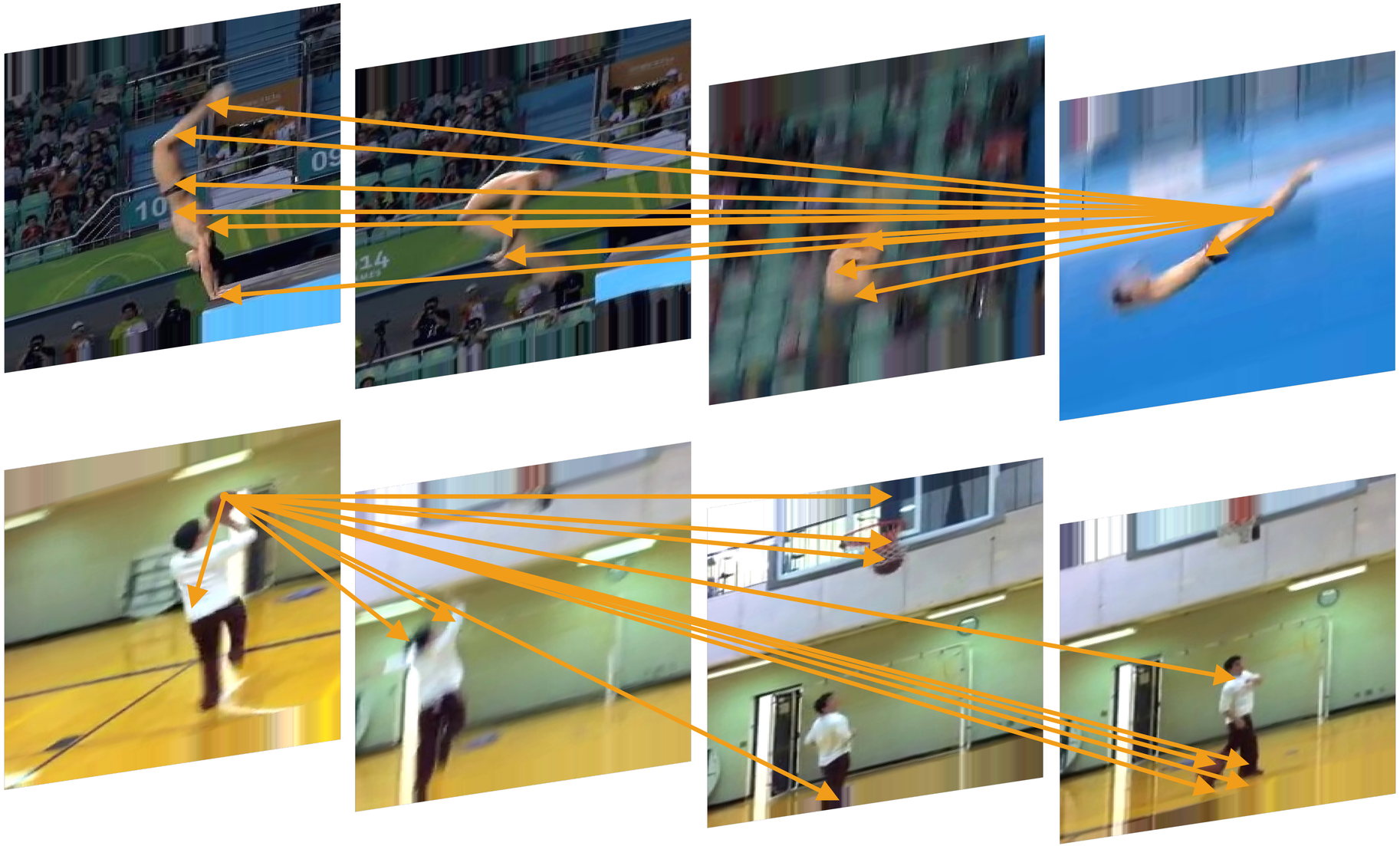


Non-local Operator as A Residual Block

$$z_i = y_i W + x_i$$



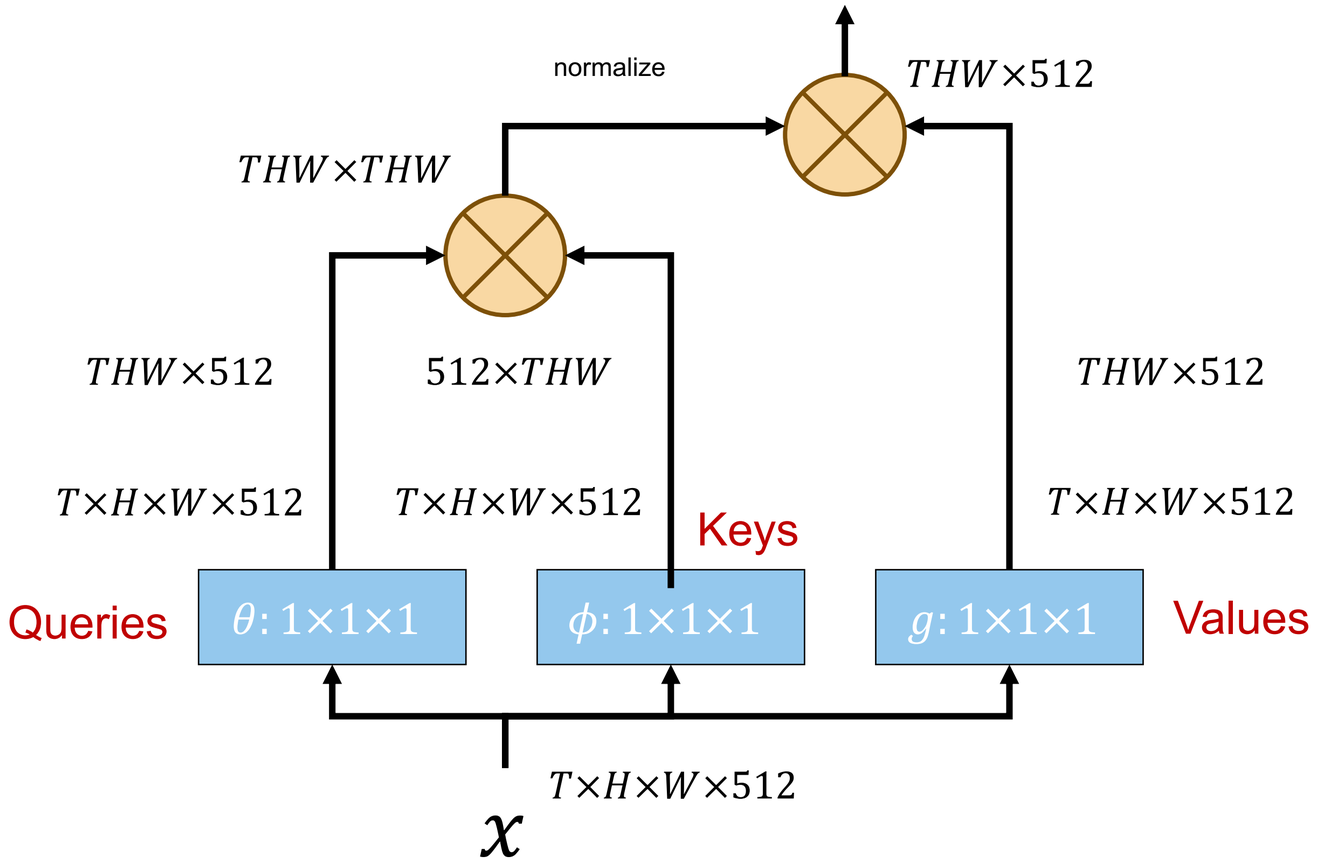
Examples



Self-Attention and Transformer for NLP

Self-Attention Operator

$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$



Self-Attention Operator

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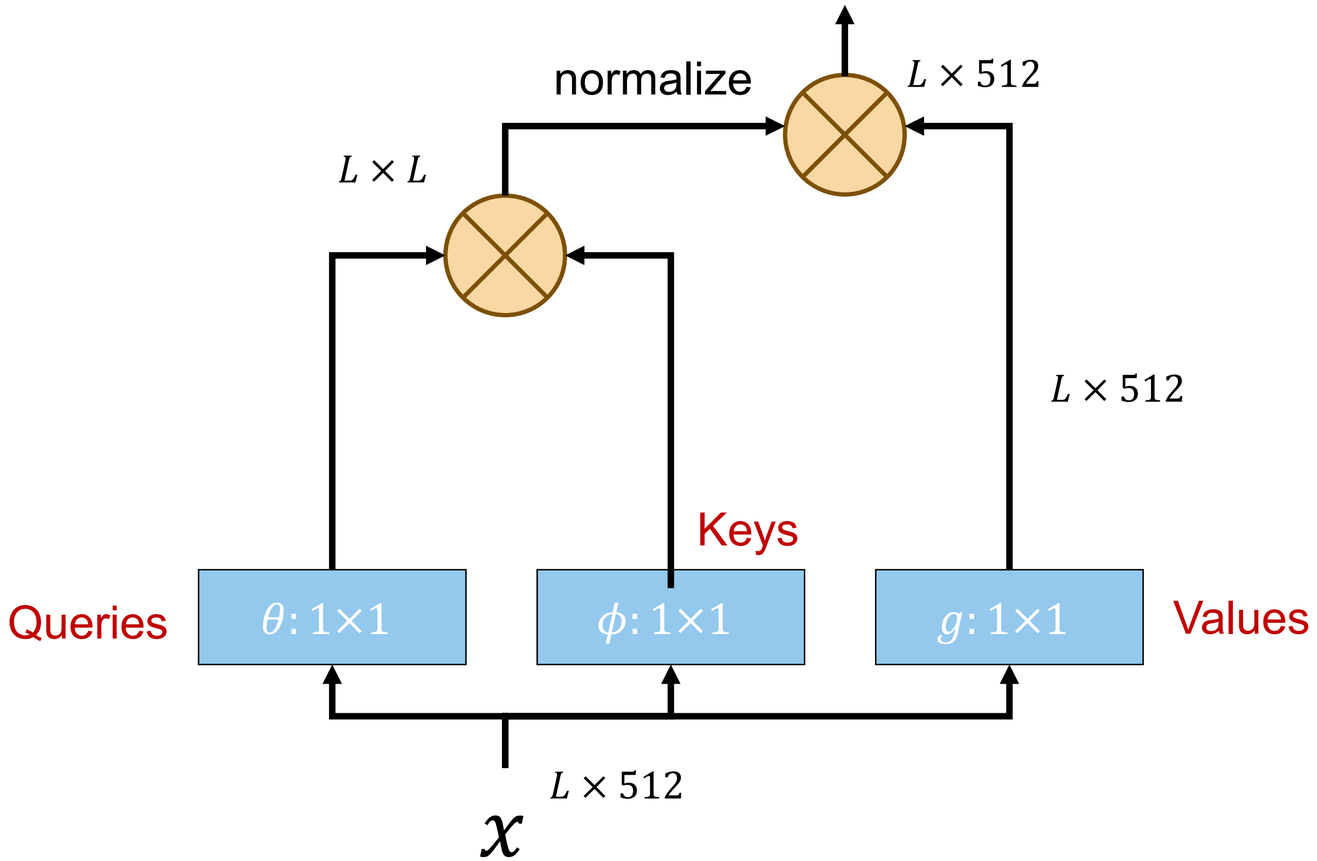

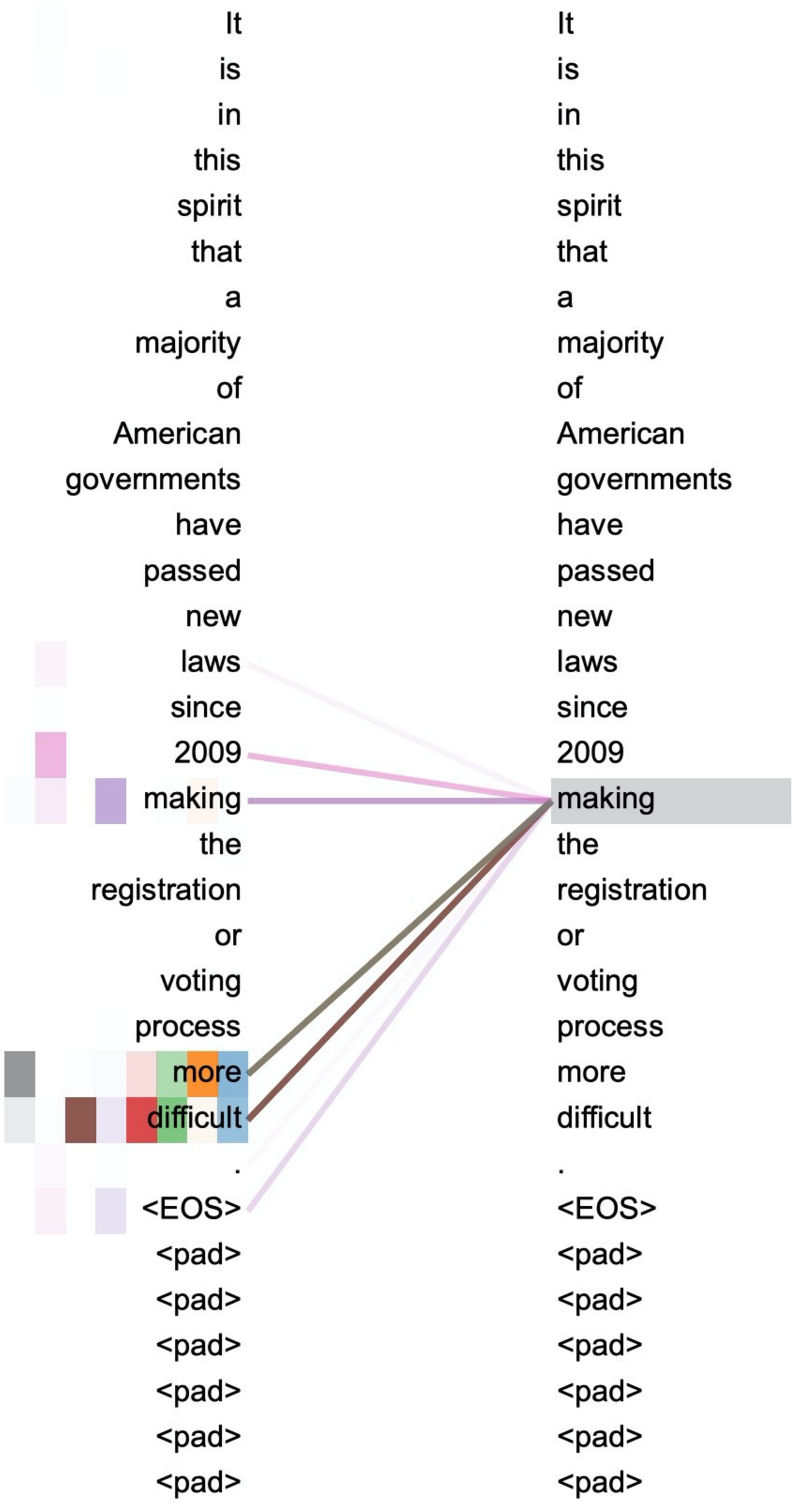
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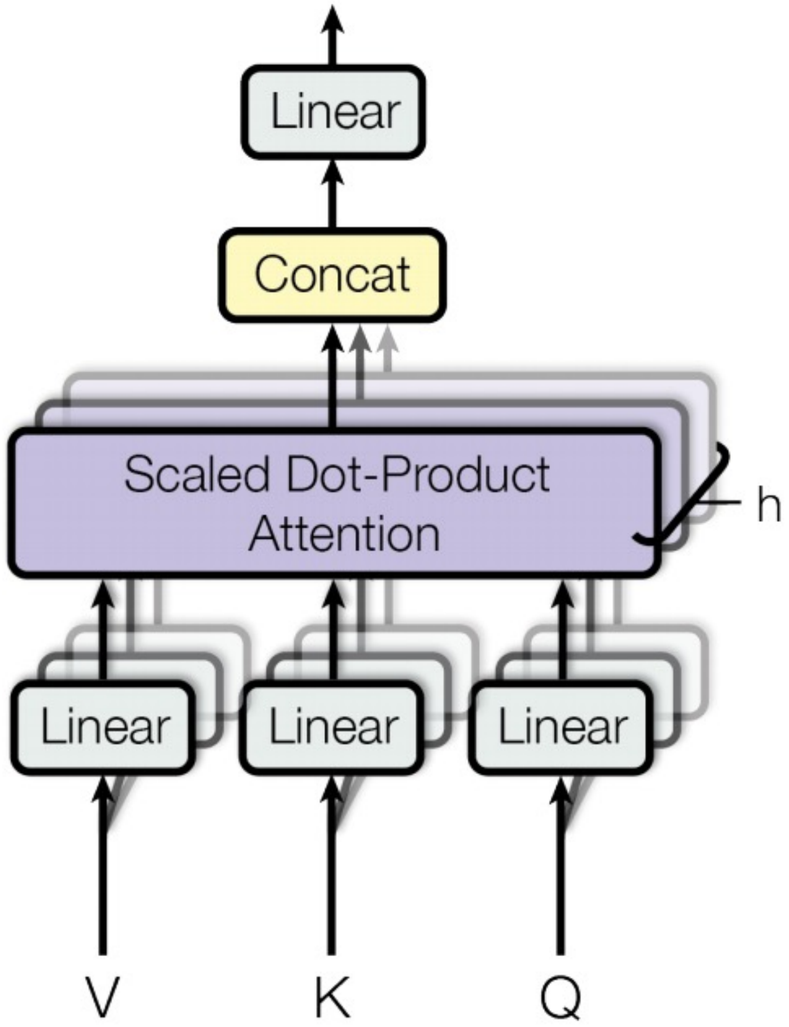
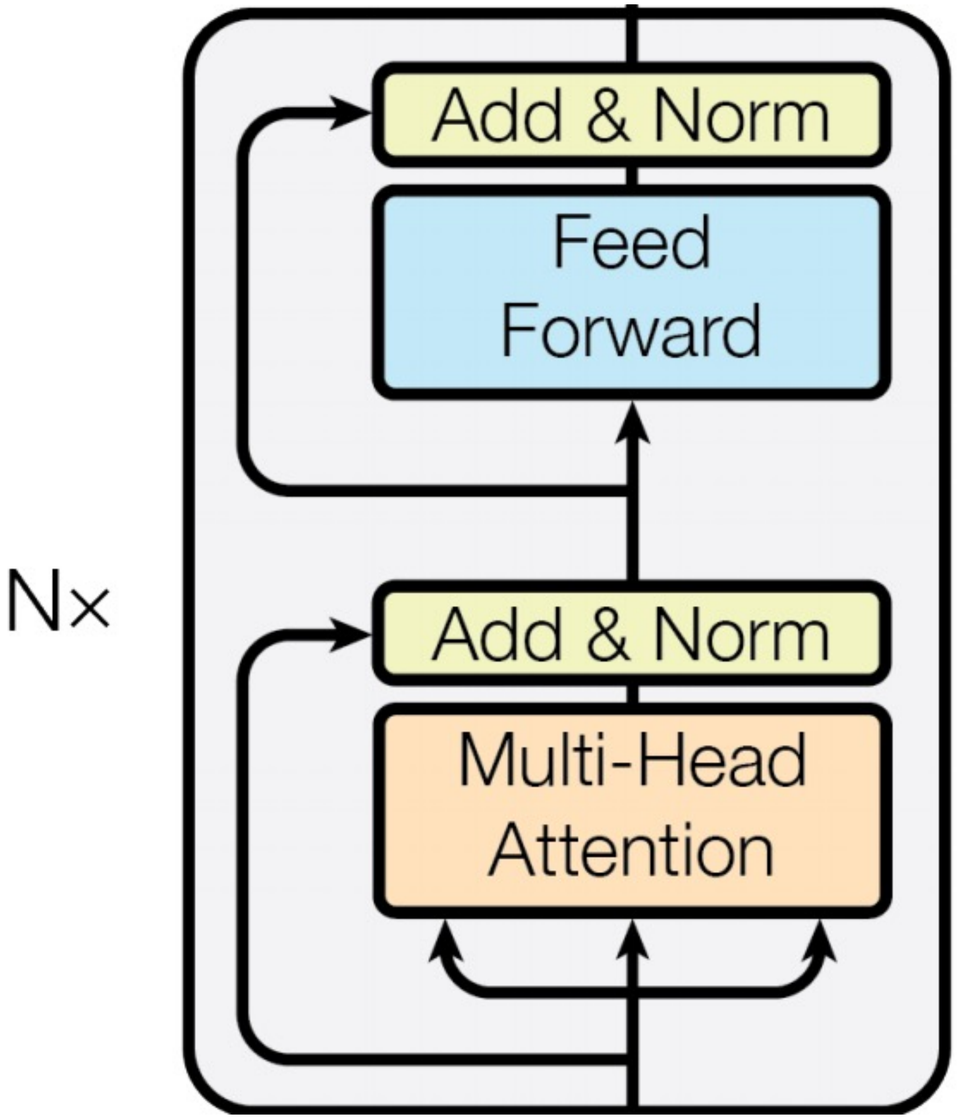
Multi-head attention

- Run h attention models in parallel on top of different linearly projected versions of Q, K, V; concatenate and linearly project the results
- Intuition: enables model to attend to different kinds of information at different positions



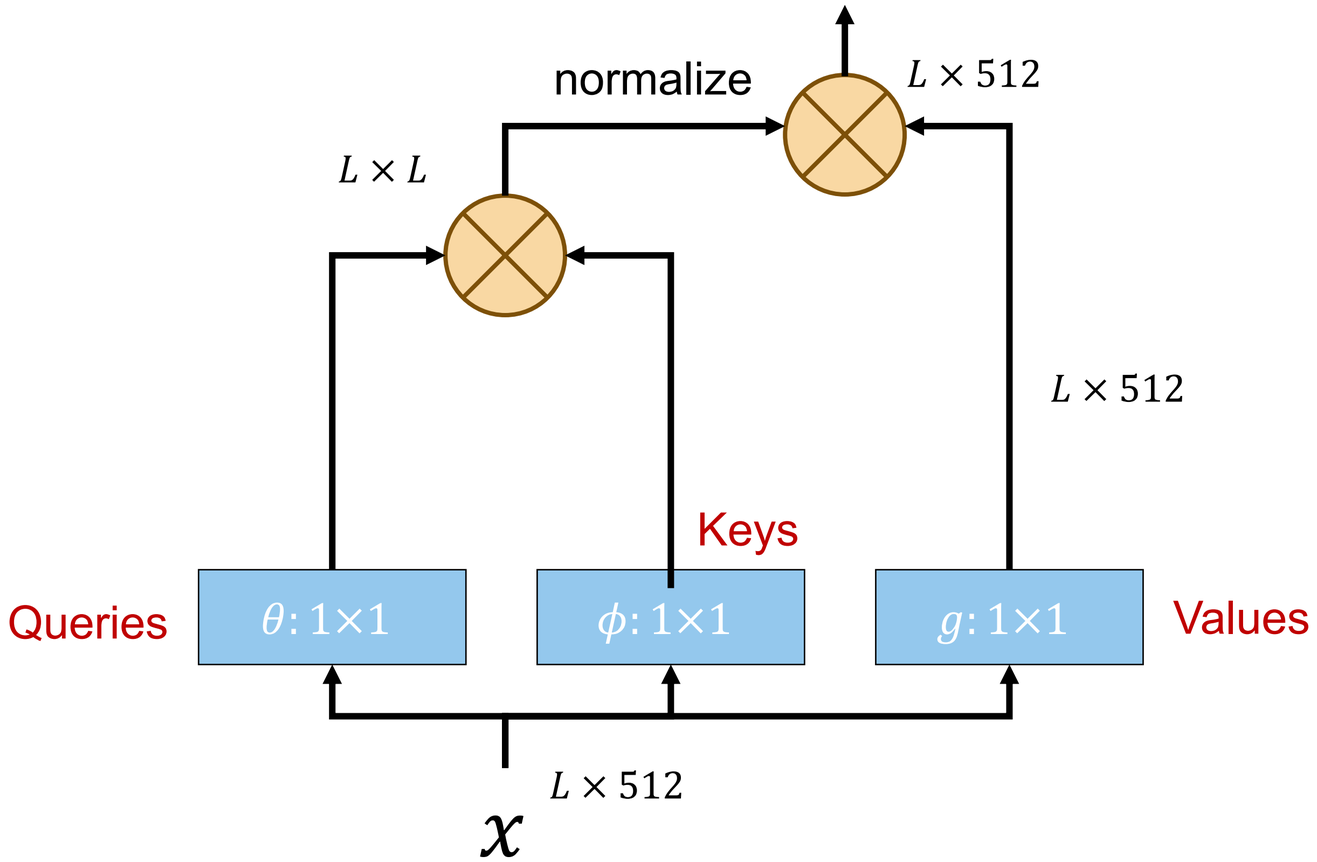
Transformer blocks

- A **Transformer** is a sequence of transformer blocks
  - Vaswani et al.: N=12 blocks, embedding dimension = 512, 6 attention heads
  - **Add & Norm:** residual connection followed by layer normalization
  - **Feedforward:** two linear layers with ReLUs in between, applied independently to each vector
- Attention is the only interaction between inputs!



Positional encoding

Self-attention does not encode the order of the inputs.



$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j) \; g(x_j)$$

Positional encoding

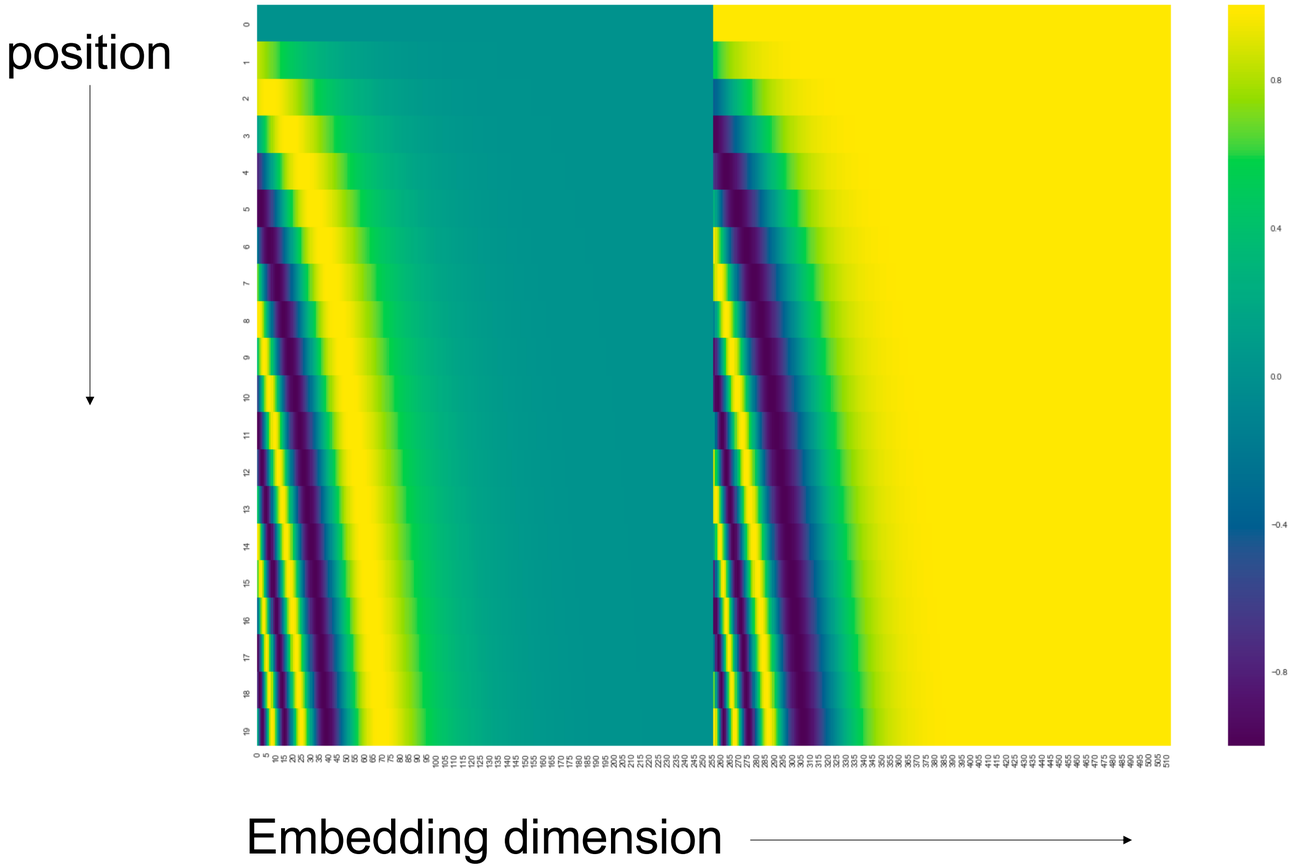
To give transformer information about ordering of tokens, add function of position (based on sines and cosines) to every input

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

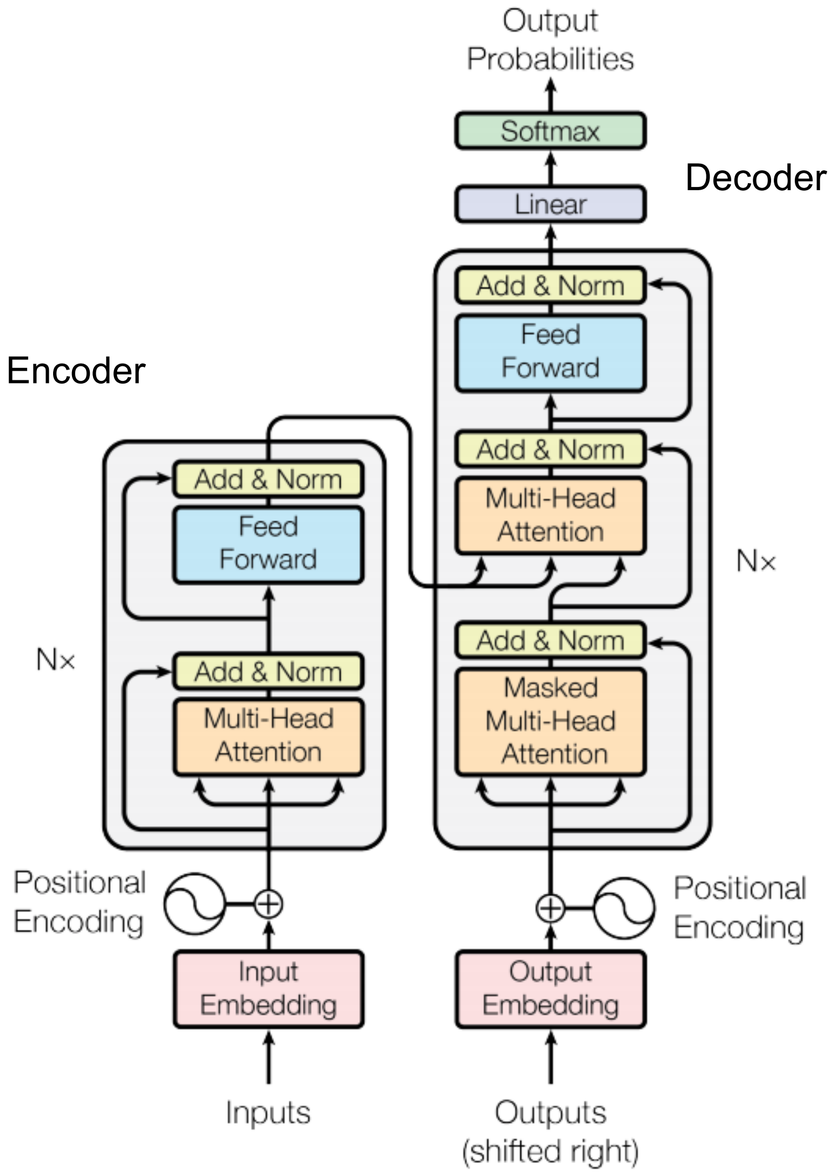
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

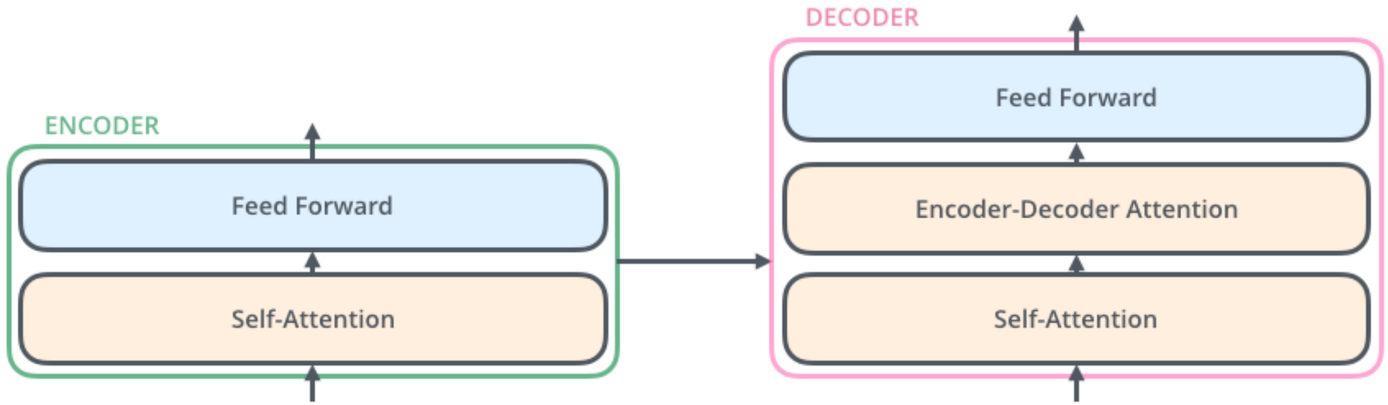
Positional encoding

To give transformer information about ordering of tokens, add function of position (based on sines and cosines) to every input



Transformer architecture: Zooming back





A. Vaswani et al., Attention is all you need, NeurIPS 2017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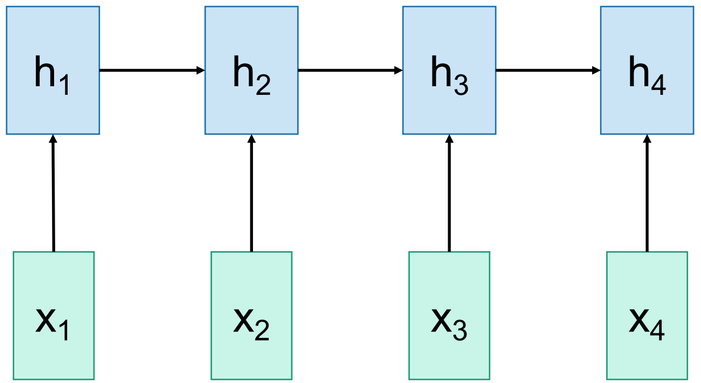
Different ways of processing sequences

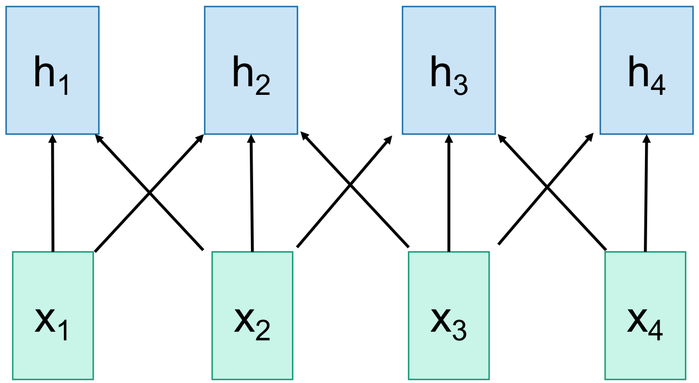
RNN



Works on **ordered sequences**

- Pros: Good at long sequences: the last hidden vector encapsulates the whole sequence
- Cons: Not parallelizable: need to compute hidden states sequentially

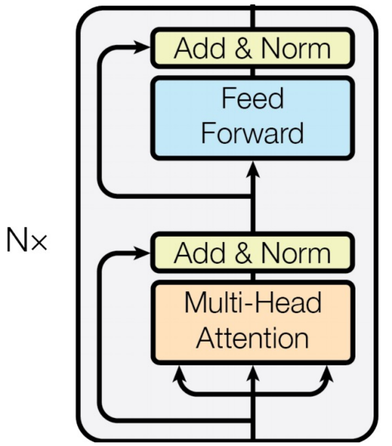
1D convolutional network



Works on **multidimensional grids**

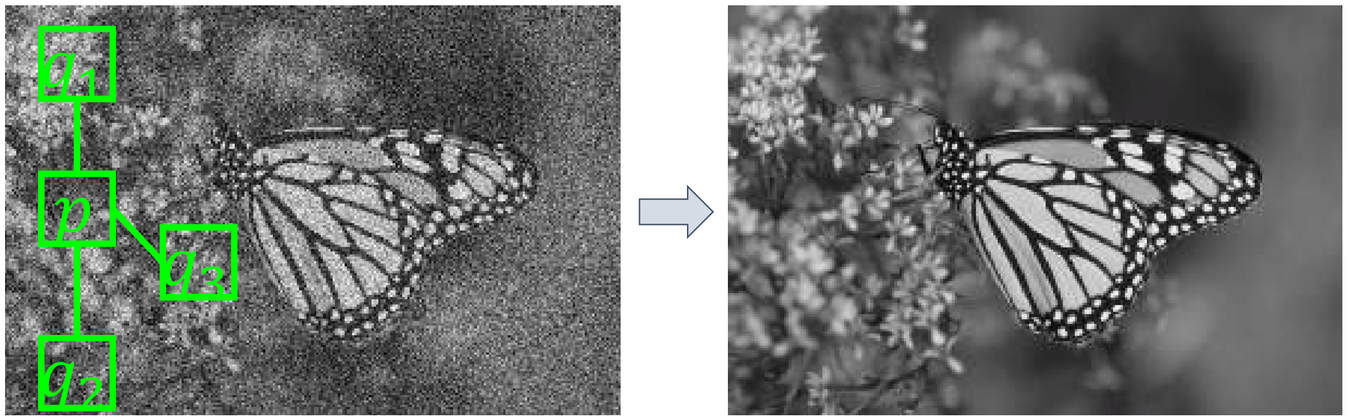
- Con: Bad at long sequences: Need to stack many conv layers for outputs to “see” the whole sequence
- Pro: Highly parallel: Each output can be computed in parallel

Transformer

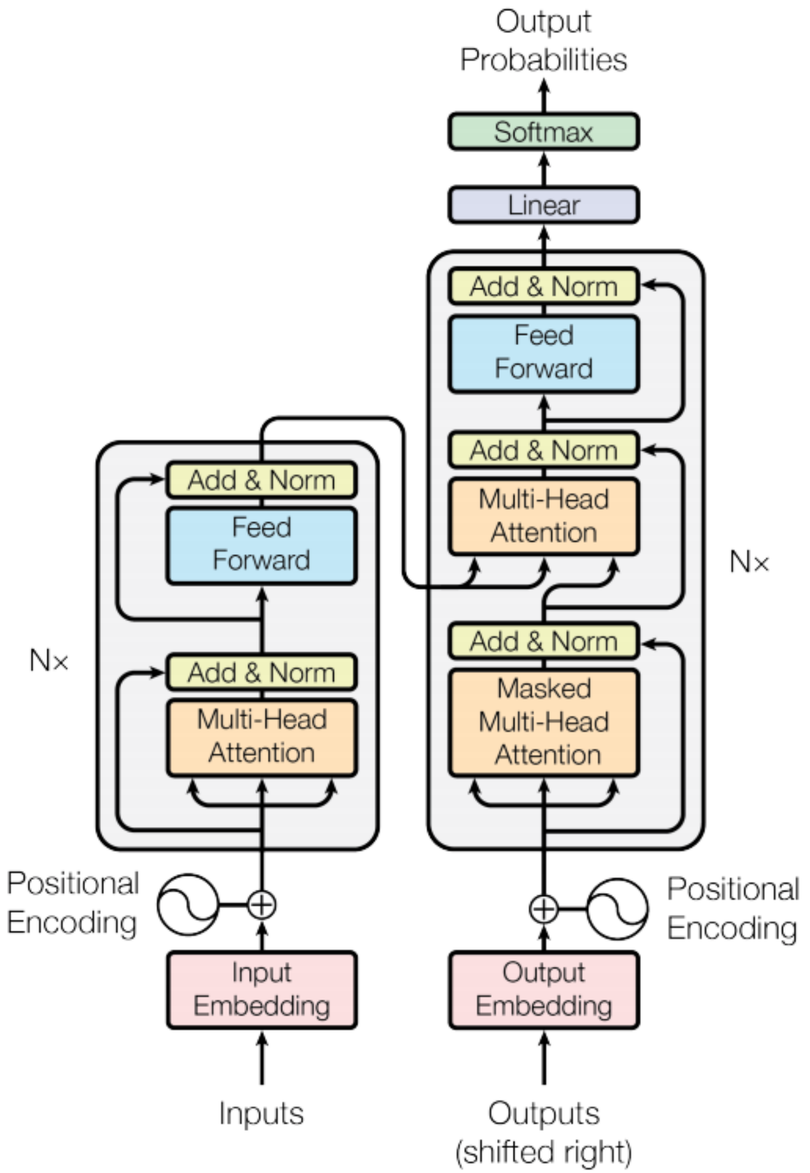


- Works on **sets of vectors**
- Pro: Good at long sequences: after one self-attention layer, each output “sees” all inputs!
- Pro: Highly parallel: Each output can be computed in parallel
- Con: Very memory-intensive

It is all Non-local Means



Buades et al., 2005.



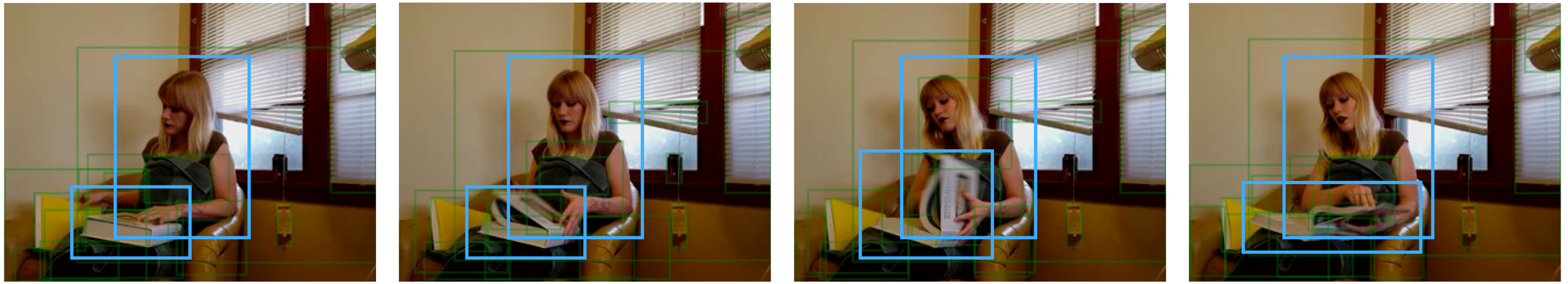
Graph Neural Networks and its connection to Self-Attention

Opening A Book

Opening A Book

The Non-local / Self-Attention Block

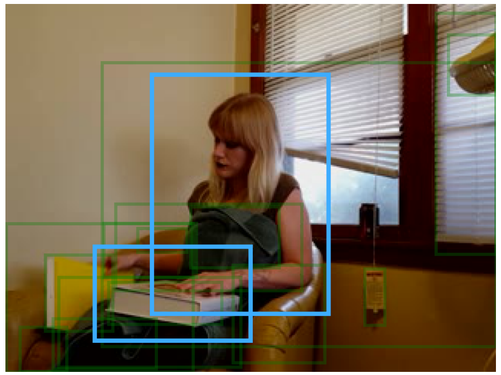
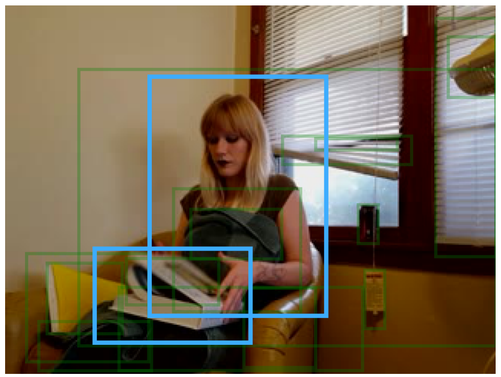
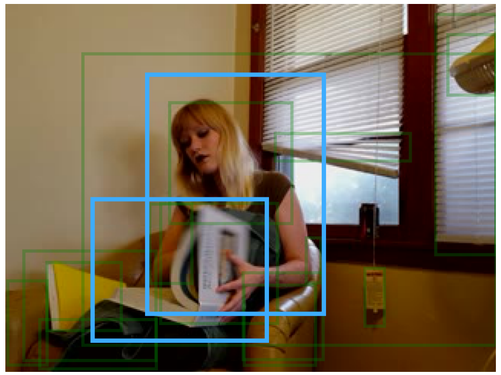
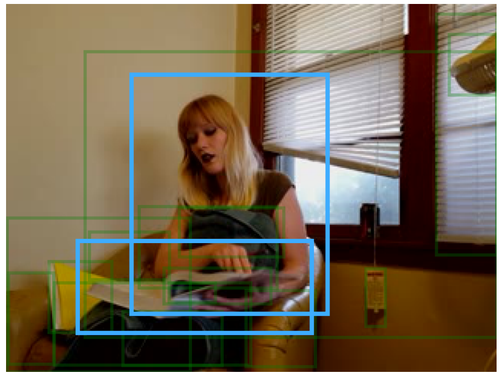
Opening A Book

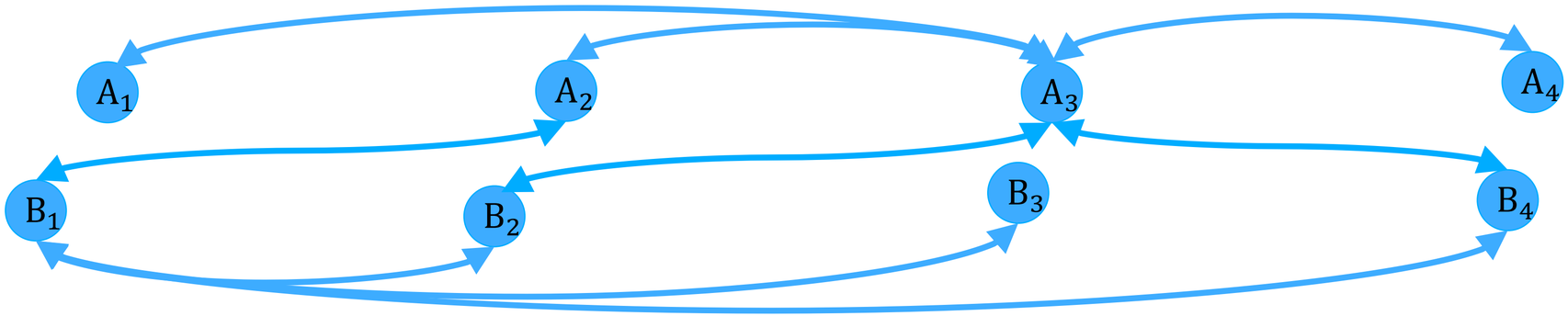


Object states changes over time

Human-object, object-object interactions

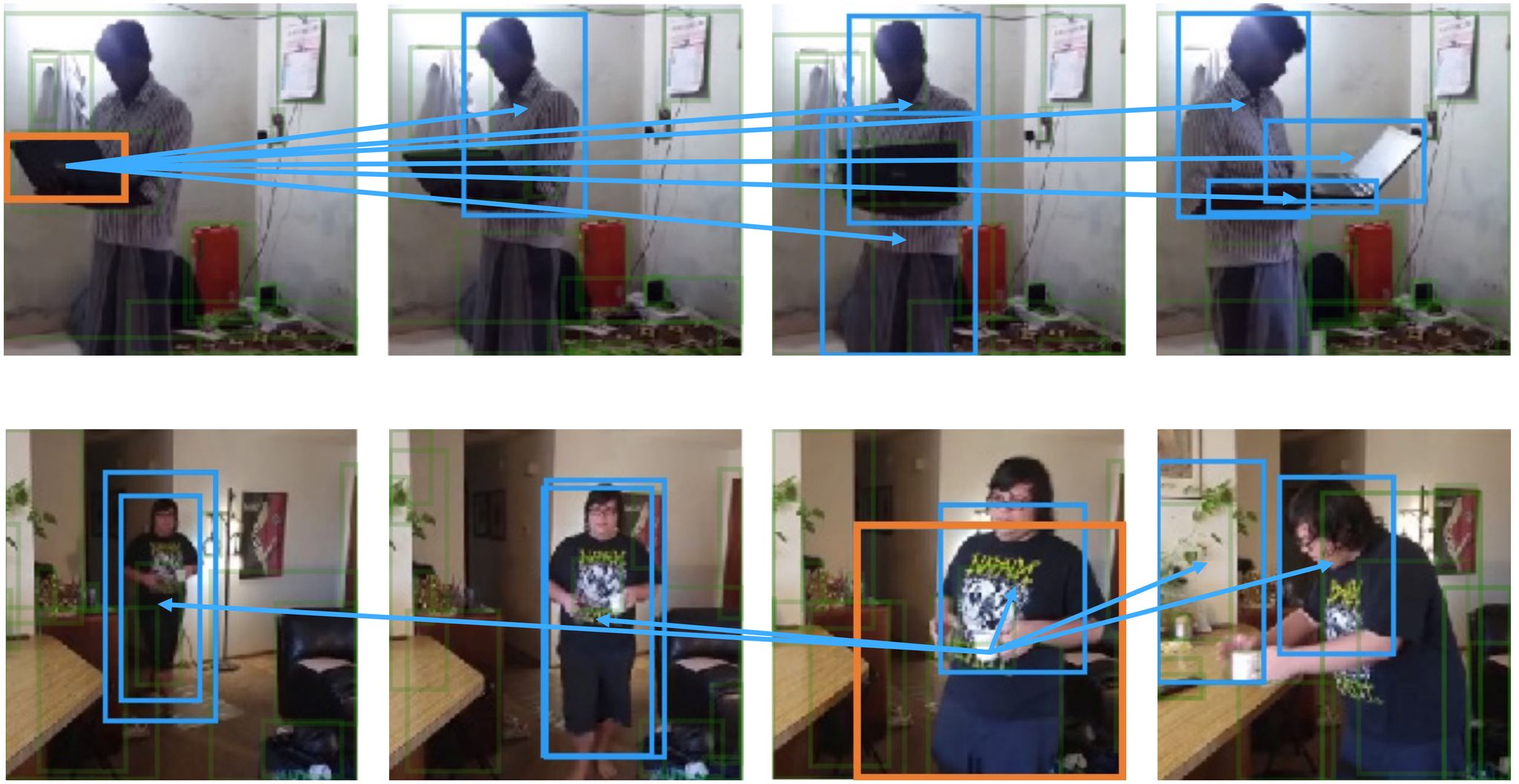
Opening A Book



Highly Correlated

Relations between Regions



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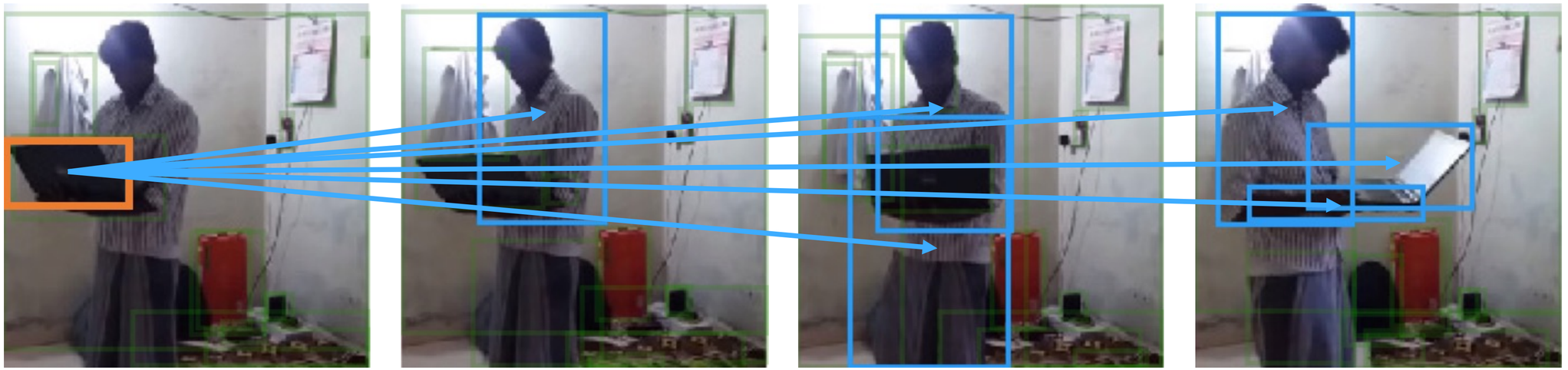
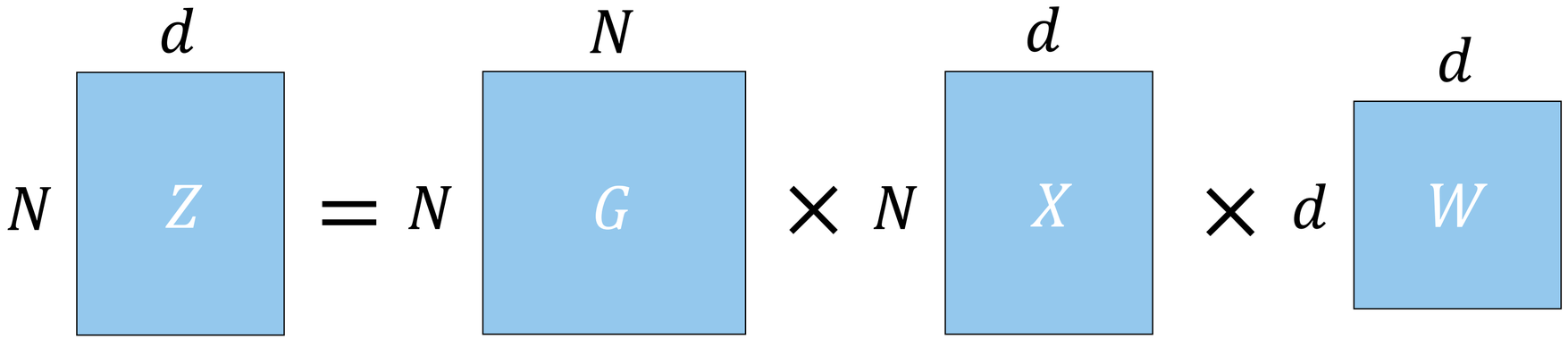


$$f(x_i, x_j) = \phi(x_i)^T \, \phi'(x_j)$$

$$G_{ij} = \frac{\exp \, f(x_i, x_j)}{\sum_{\forall j} \exp \, f(x_i, x_j)}$$

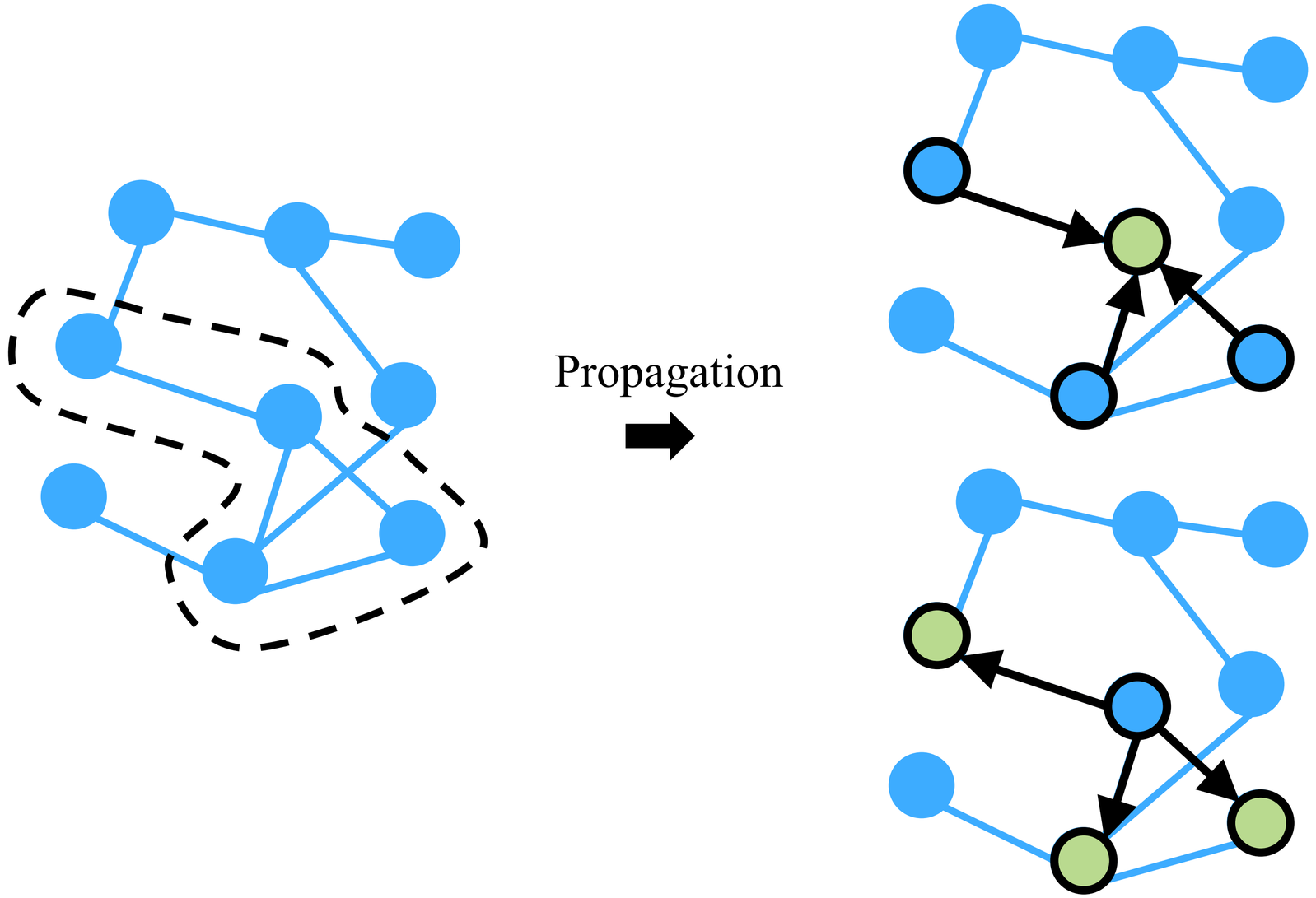
Graph Convolutional Network

$$Z = GXW$$



Kipf et al., 2017

Graph Convolutional Network



Connecting Non-local Means and GCN

The Non-local Operator:

$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$

$$= \sum_{\forall j} \frac{f(x_i, x_j)}{\sum_{\forall j} f(x_i, x_j)} g(x_j)$$

$$= \sum_{\forall j} G_{ij}\ g(x_j)$$

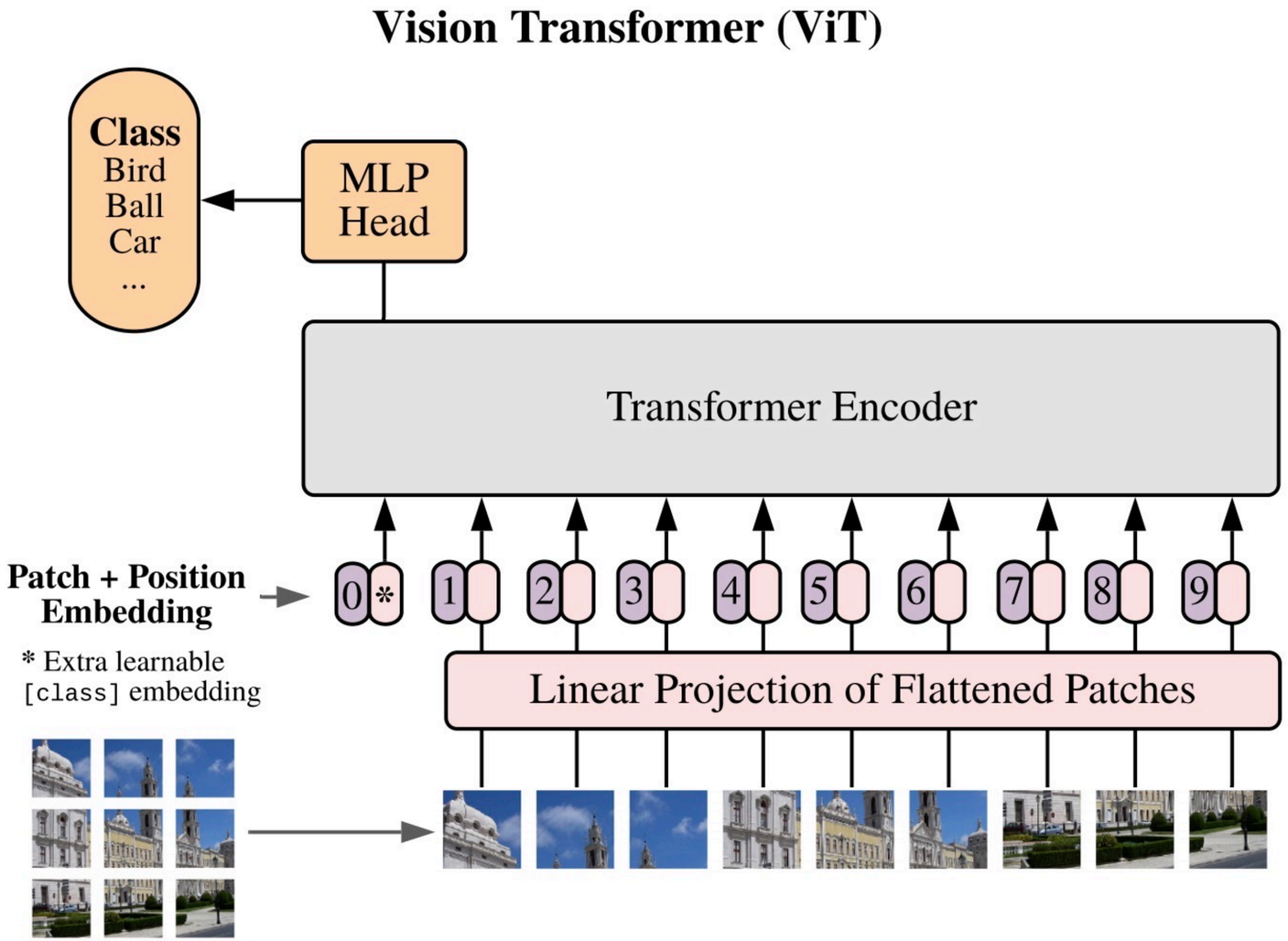
$$z_i = y_i W + x_i$$

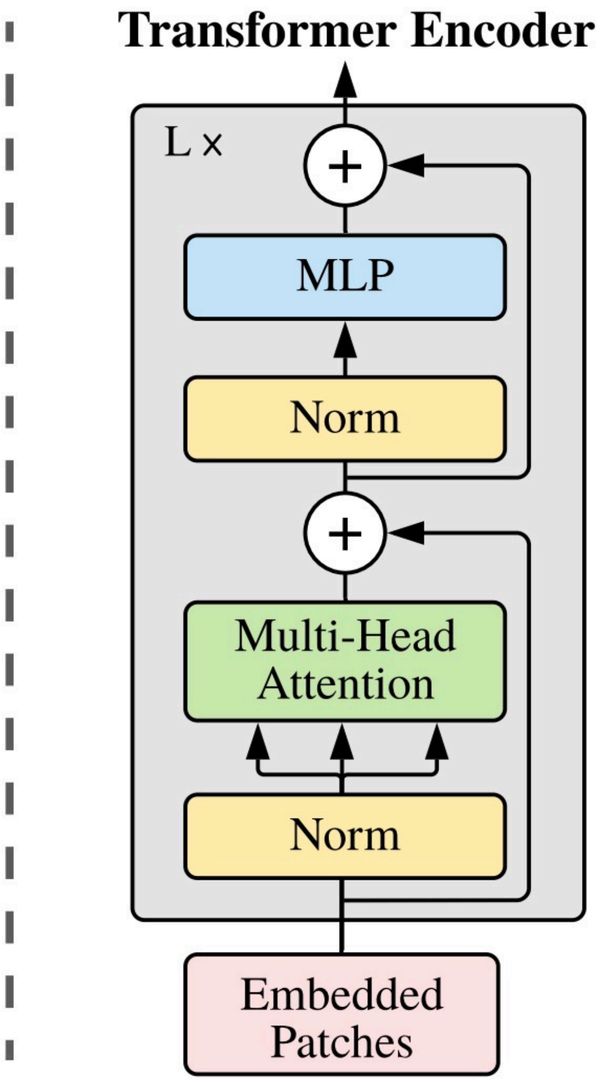
$$= \sum_{\forall j} G_{ij}\ g(x_j)\, W + x_i$$

$$Z = G\ g(X)\ W + X$$

The Graph Convolution

Vision Transformer (ViT) [Dosovitskiy et al. 2021]





This Class

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- Self-Attention and Transformer for NLP
- Graph Neural Networks