Self-Attention, Transformer, and Graph Networks

Xiaolong Wang

Previous classes

- RNN for time sequence processing

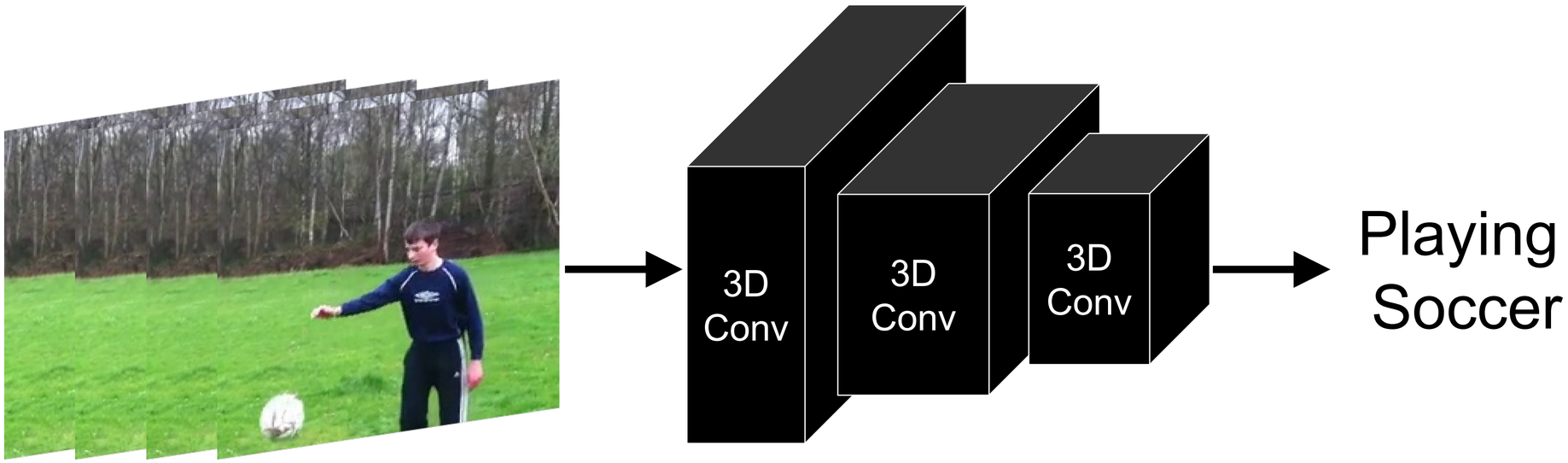
- Video understanding with temporal convolution, 3D CNN

This Class

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

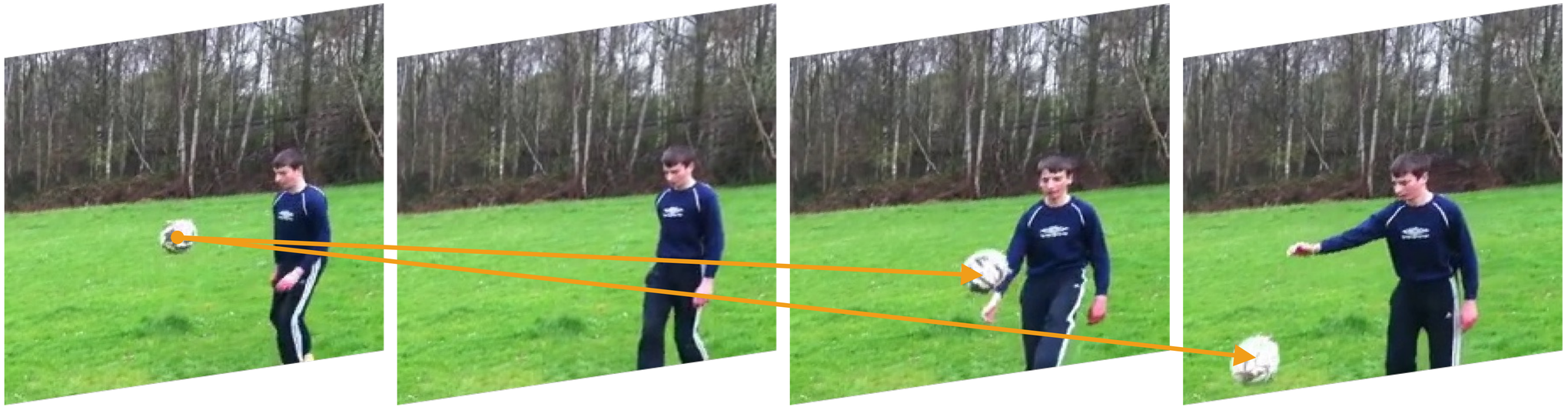
Non-local Neural Network for Videos

Video Recognition



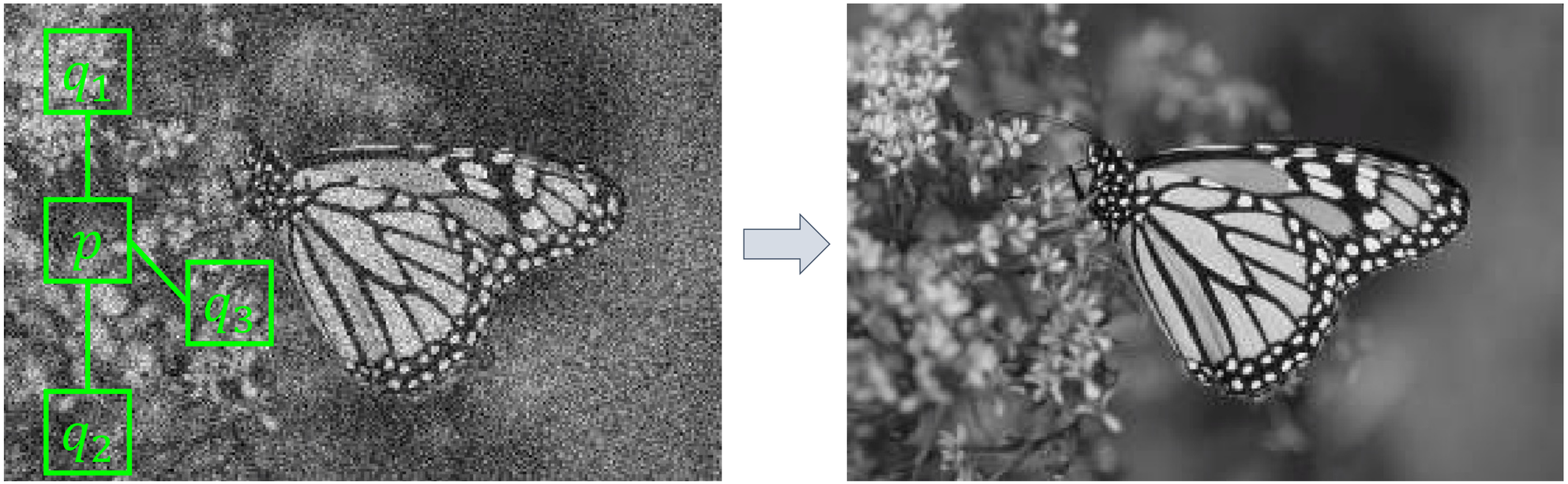
Reasoning for Action Recognition

Long-rang explicit reasoning



Wang et al., 2018.

Non-local Means

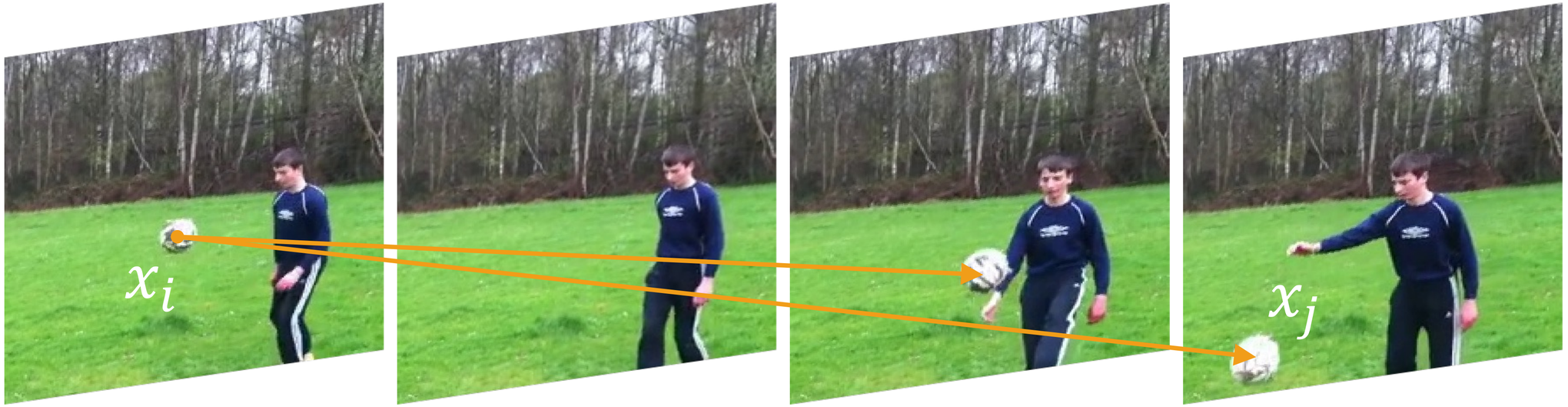


Buades et al., 2005.

Non-local Operator

Operation in feature space

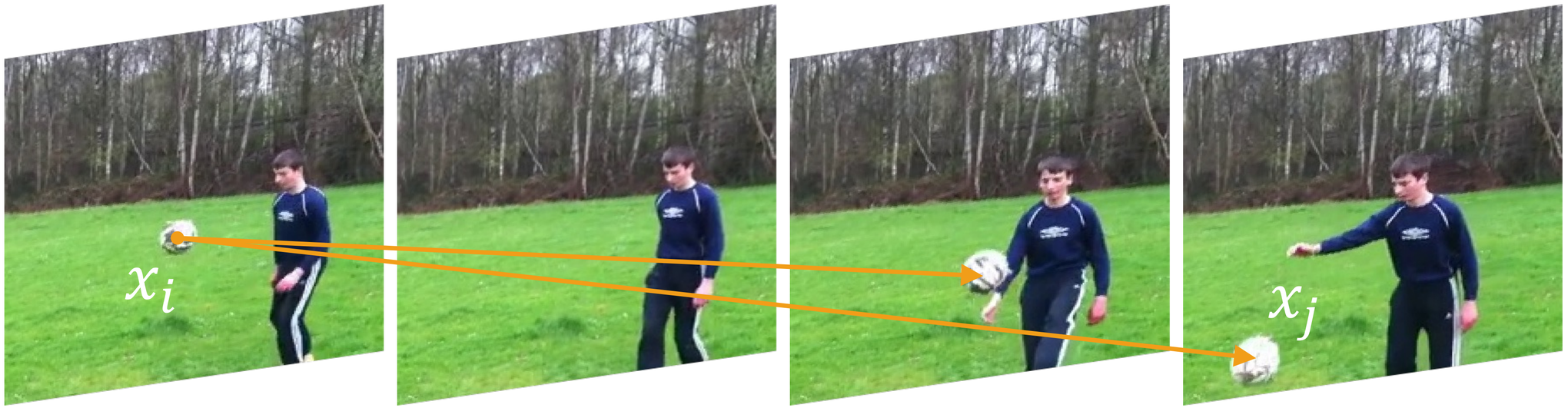
Can be embedded into any ConvNets



Non-local Operator

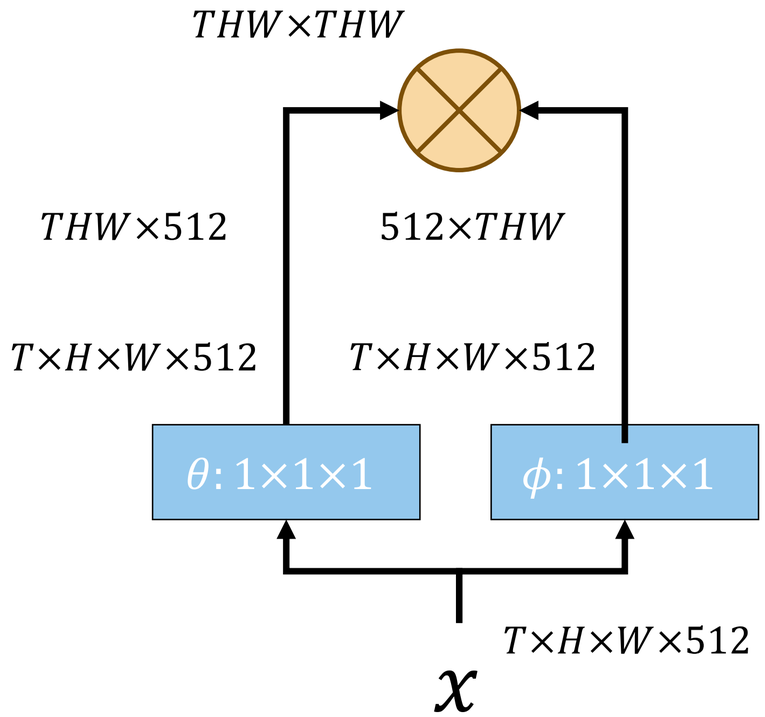
$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j) \; g(x_j)$$

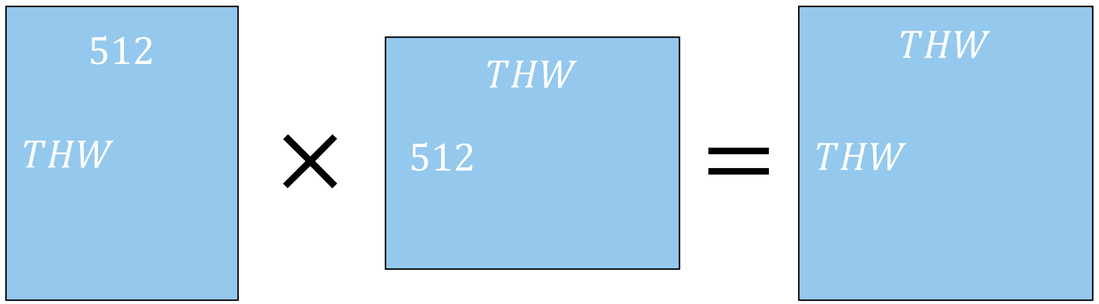
Affinity Features



Non-local Operator

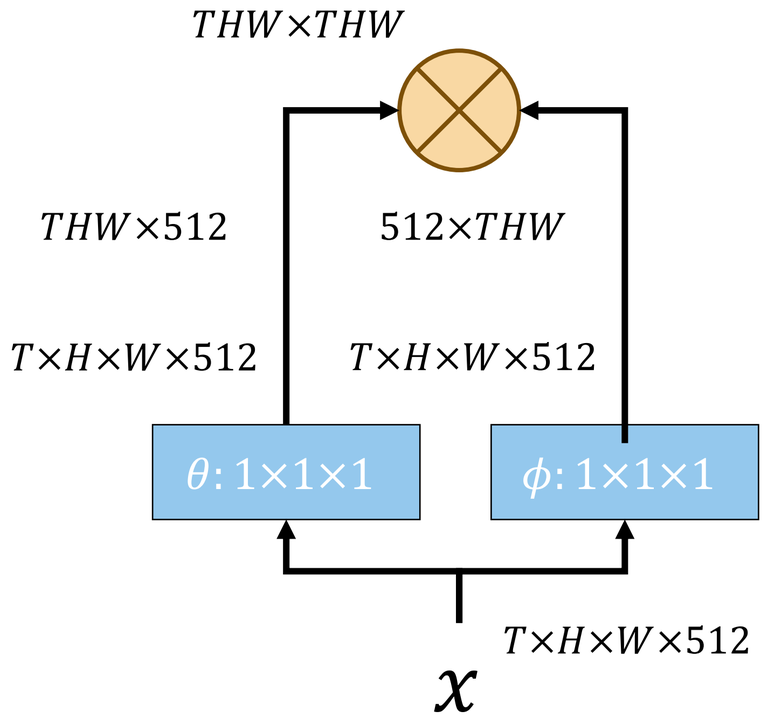
$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$

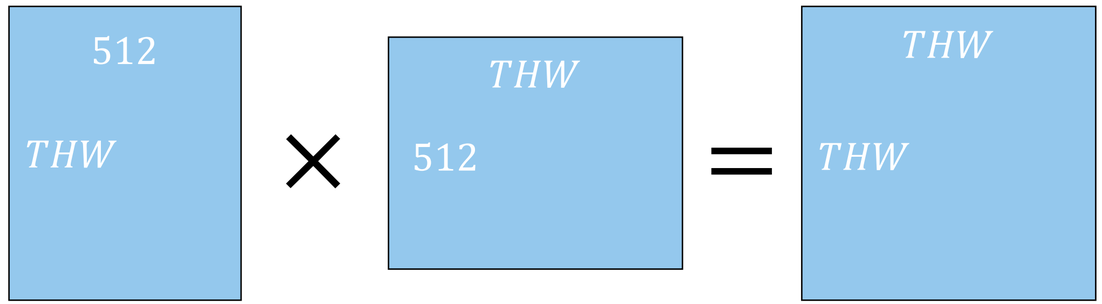




Non-local Operator

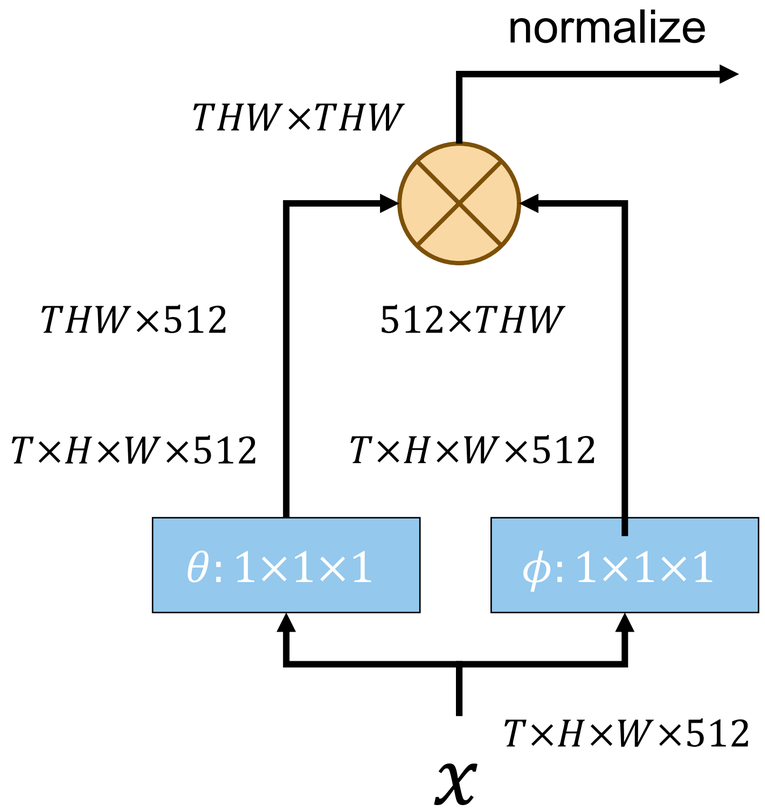
$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$





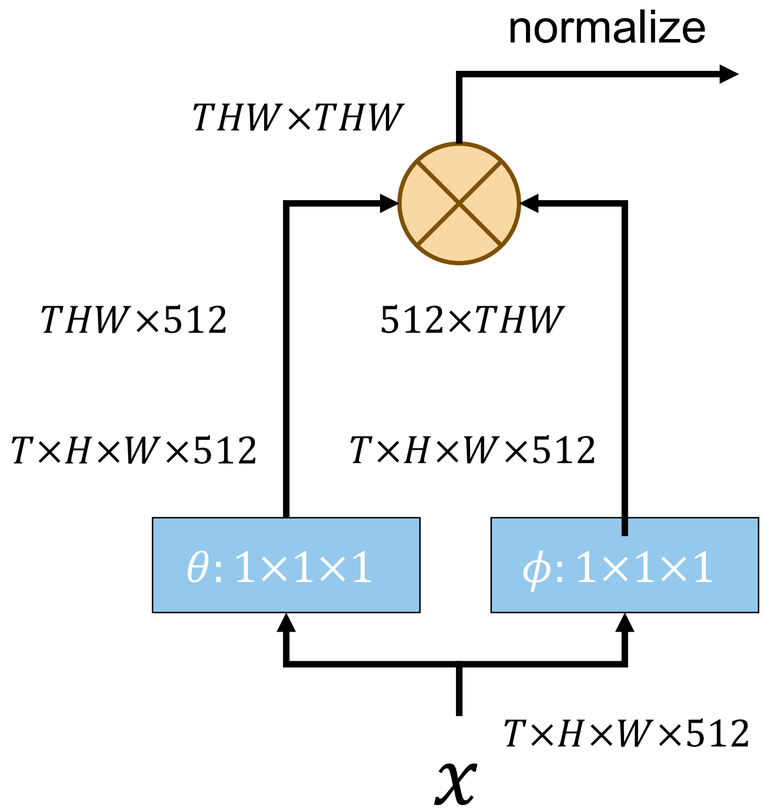
Non-local Operator

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



Non-local Operator

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



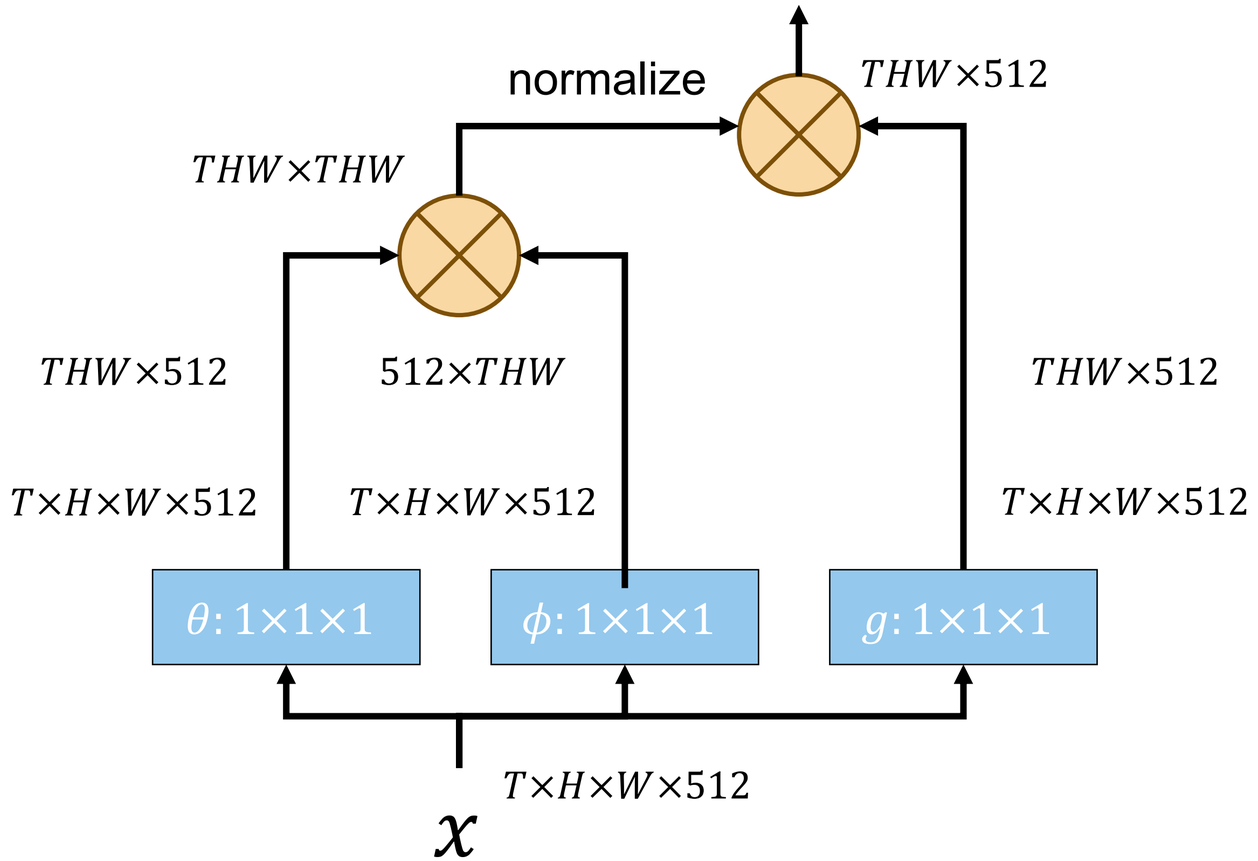
$$f\left(x_i, x_j\right) = \exp(x_i^T x_j)$$

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

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

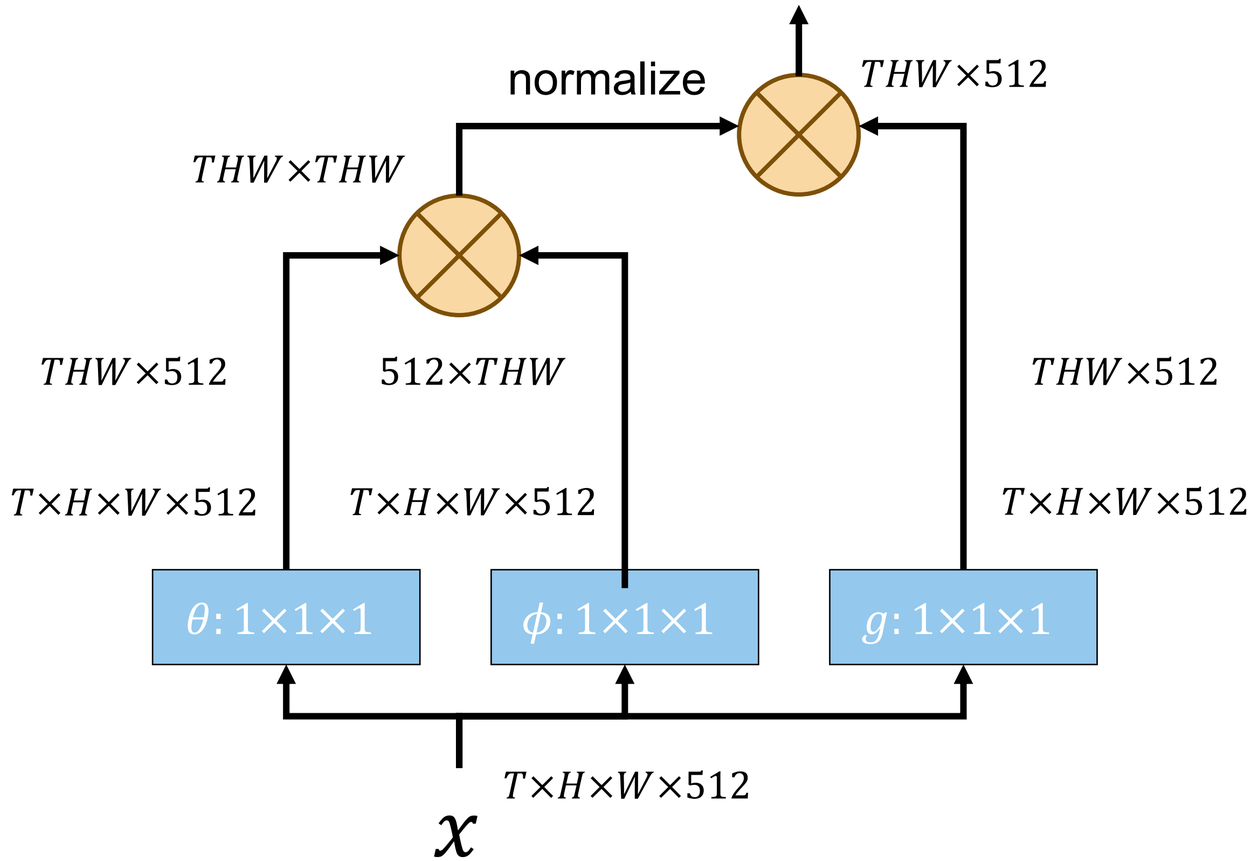
Non-local Operator

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



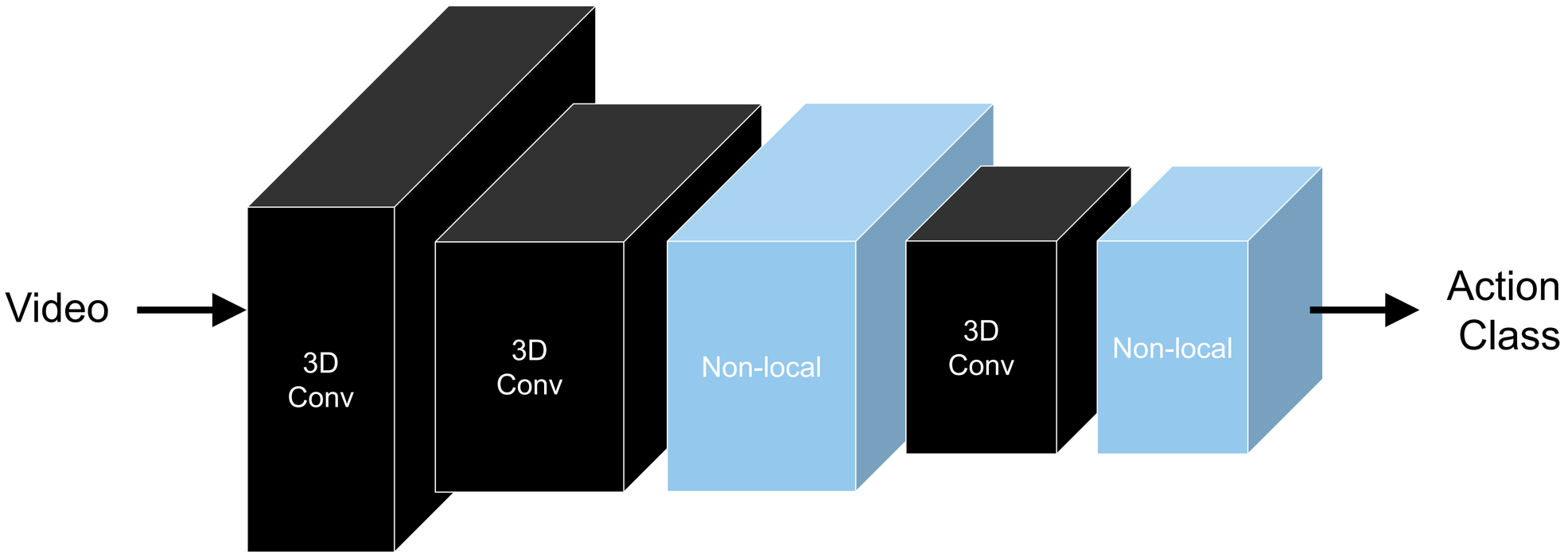
Non-local Operator

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

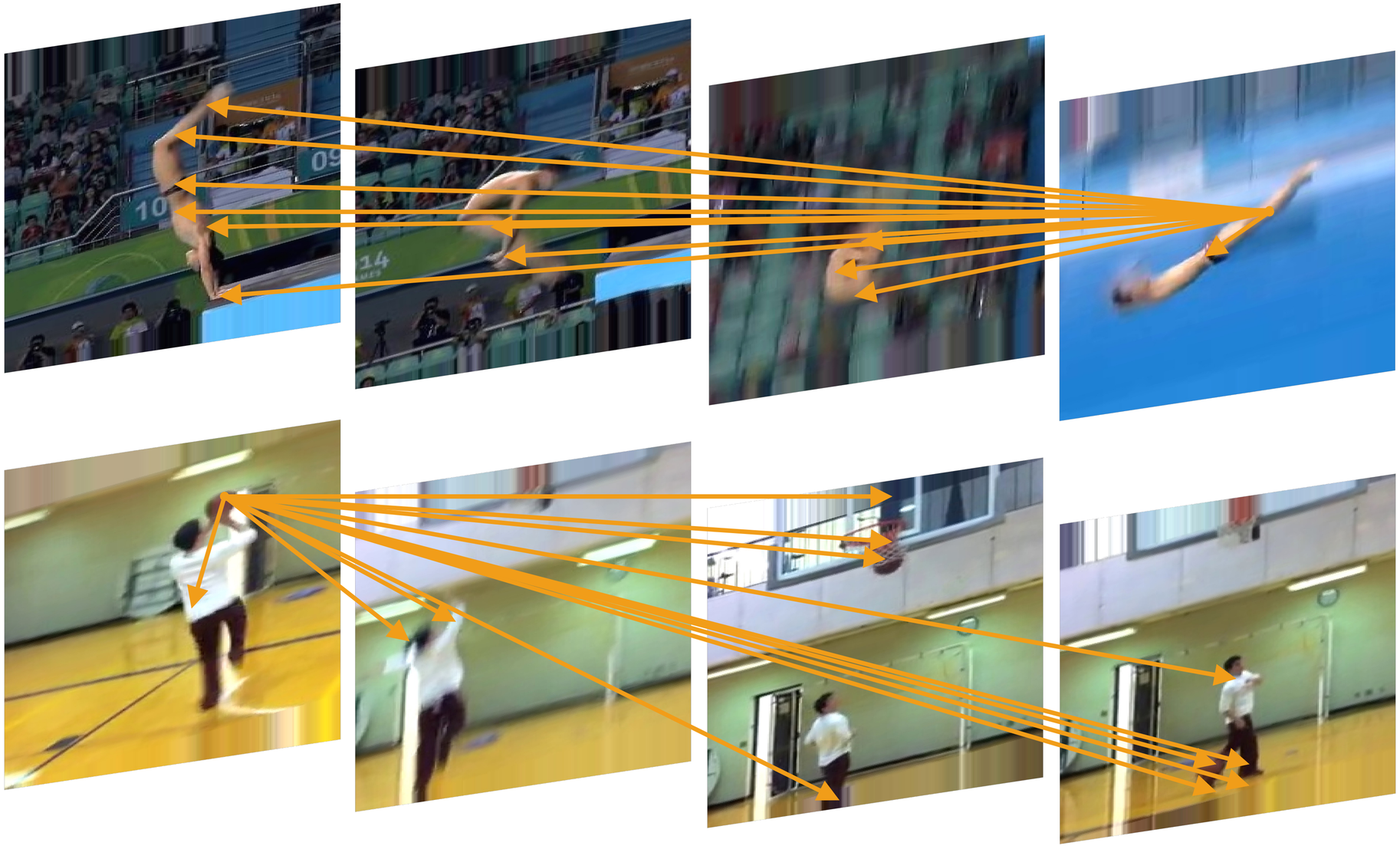


Non-local Operator as A Residual Block

$$z_i = y_i W + x_i$$



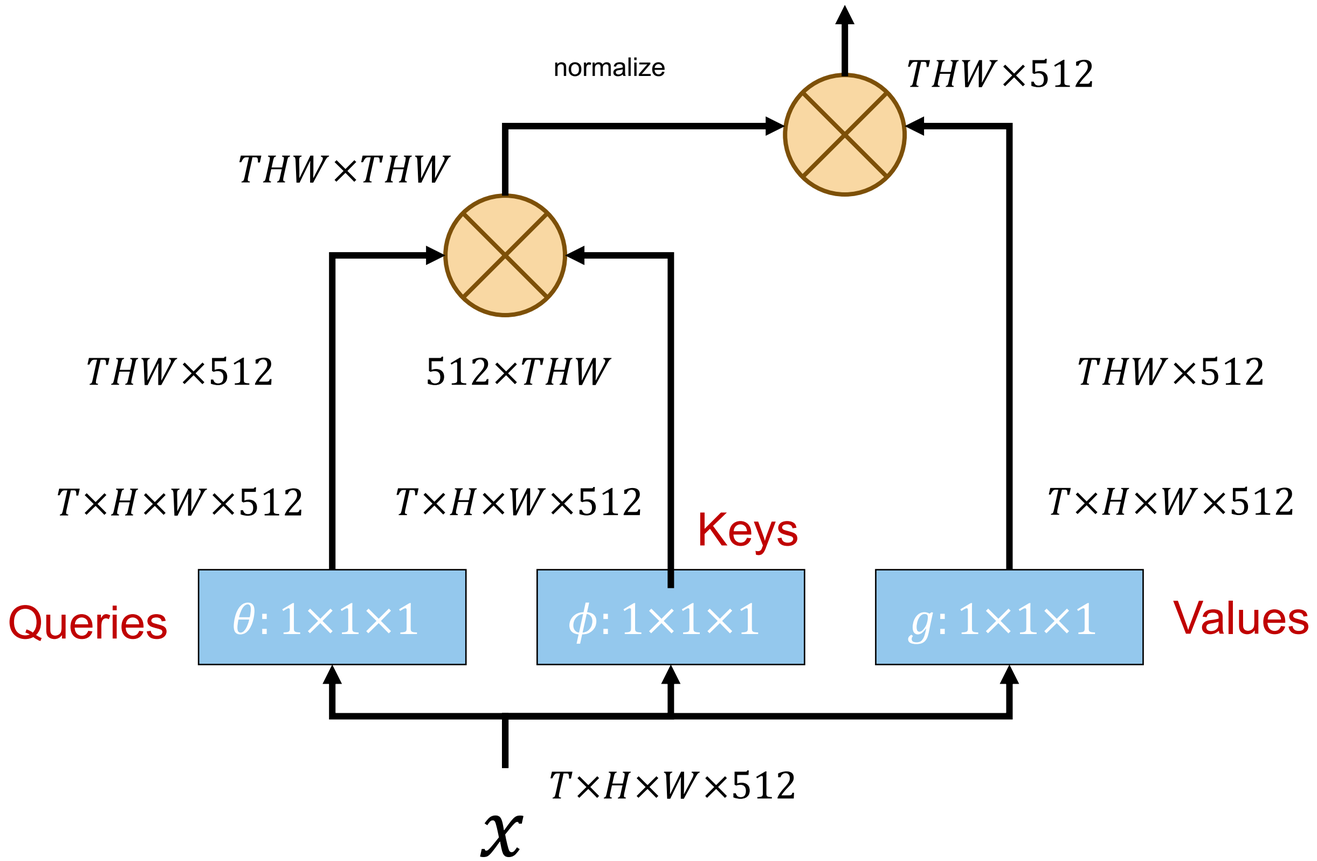
Examples



Self-Attention and Transformer for NLP

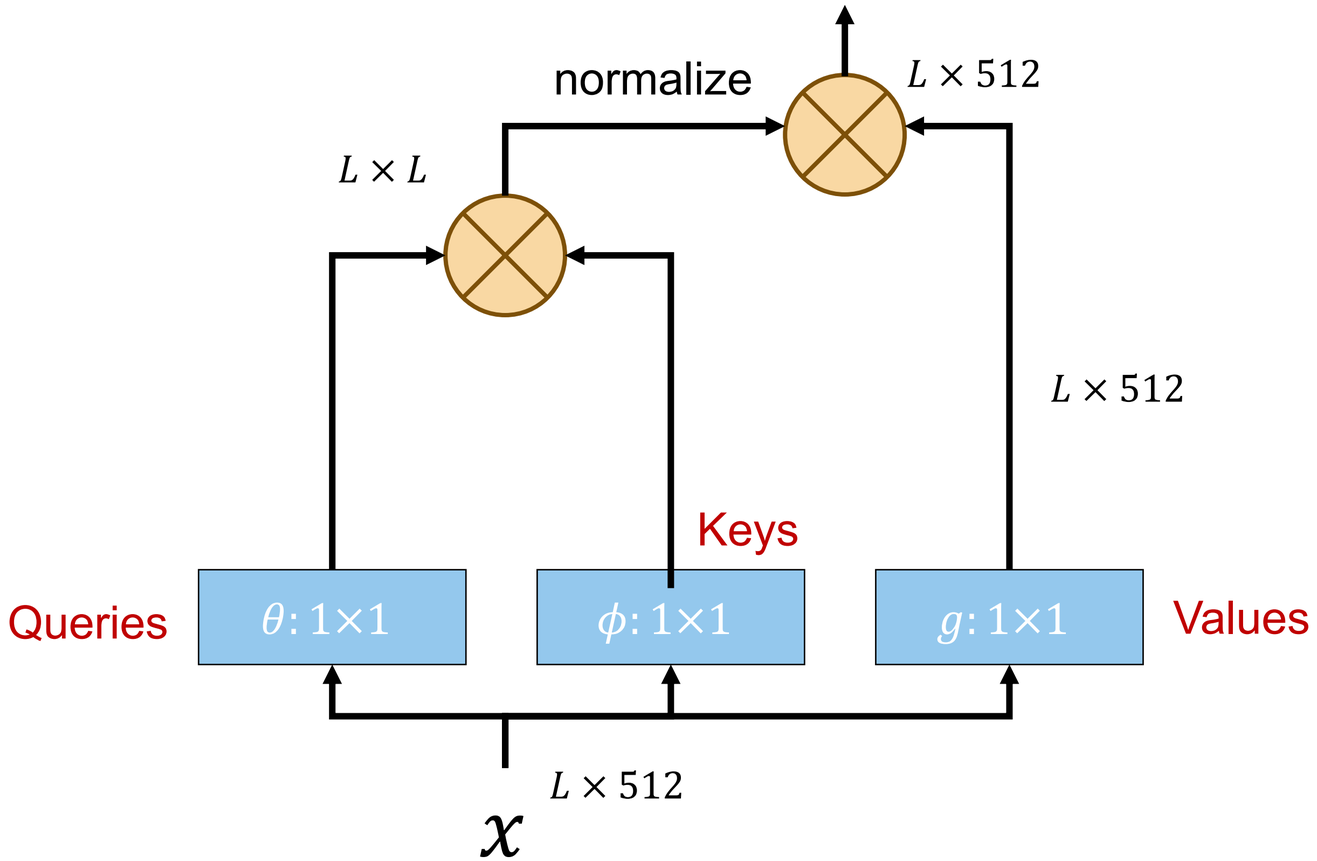
Self-Attention Operator

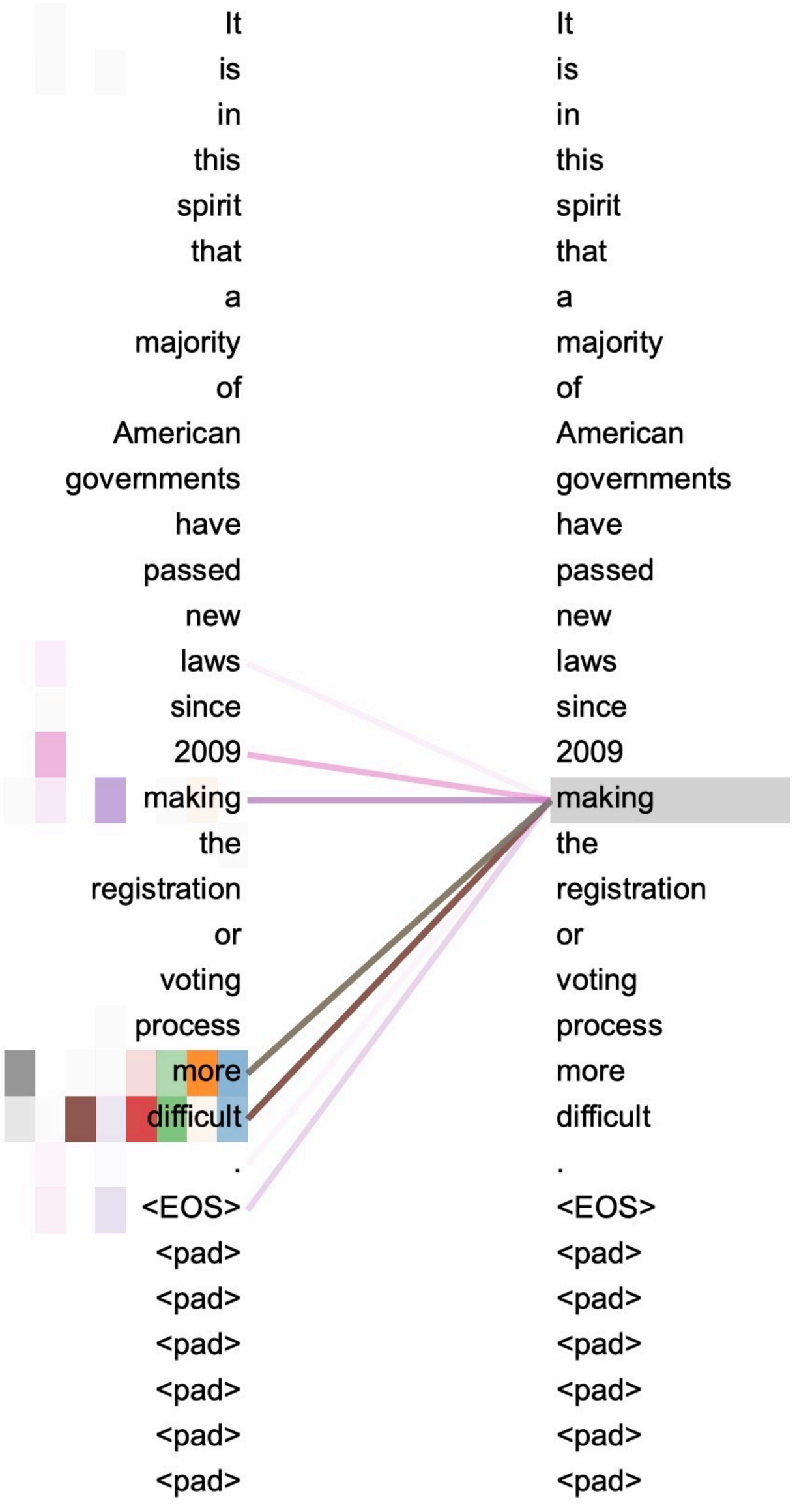
$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$



Self-Attention Operator

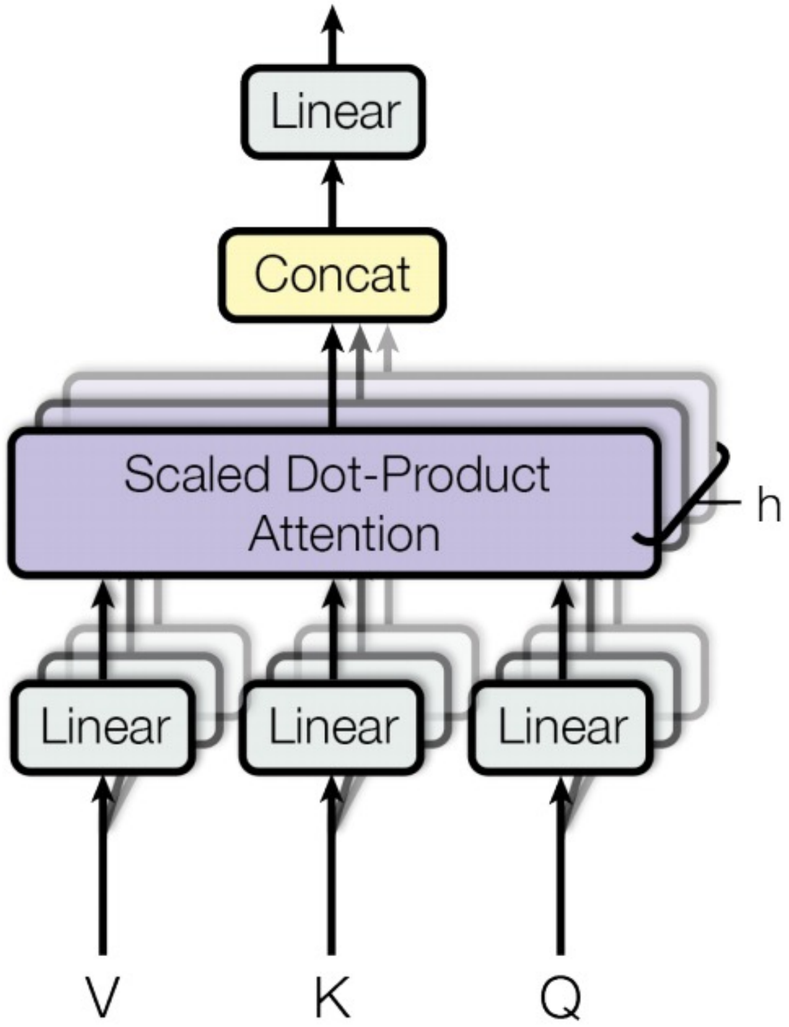
$$y_i = \frac{1}{C(x)} \sum_{\forall j} f(x_i, x_j)\ g(x_j)$$




It
is
in
this
spirit
that
a
majority
of
American
governments
have
passed
new
laws
since
2009
making
the
registration
or
voting
process
more
difficult
.
<EOS>
<pad>
<pad>
<pad>
<pad>
<pad>
<pad>
It
is
in
this
spirit
that
a
majority
of
American
governments
have
passed
new
laws
since
2009
making
the
registration
or
voting
process
more
difficult
.
<EOS>
<pad>
<pad>
<pad>
<pad>
<pad>
<pad>

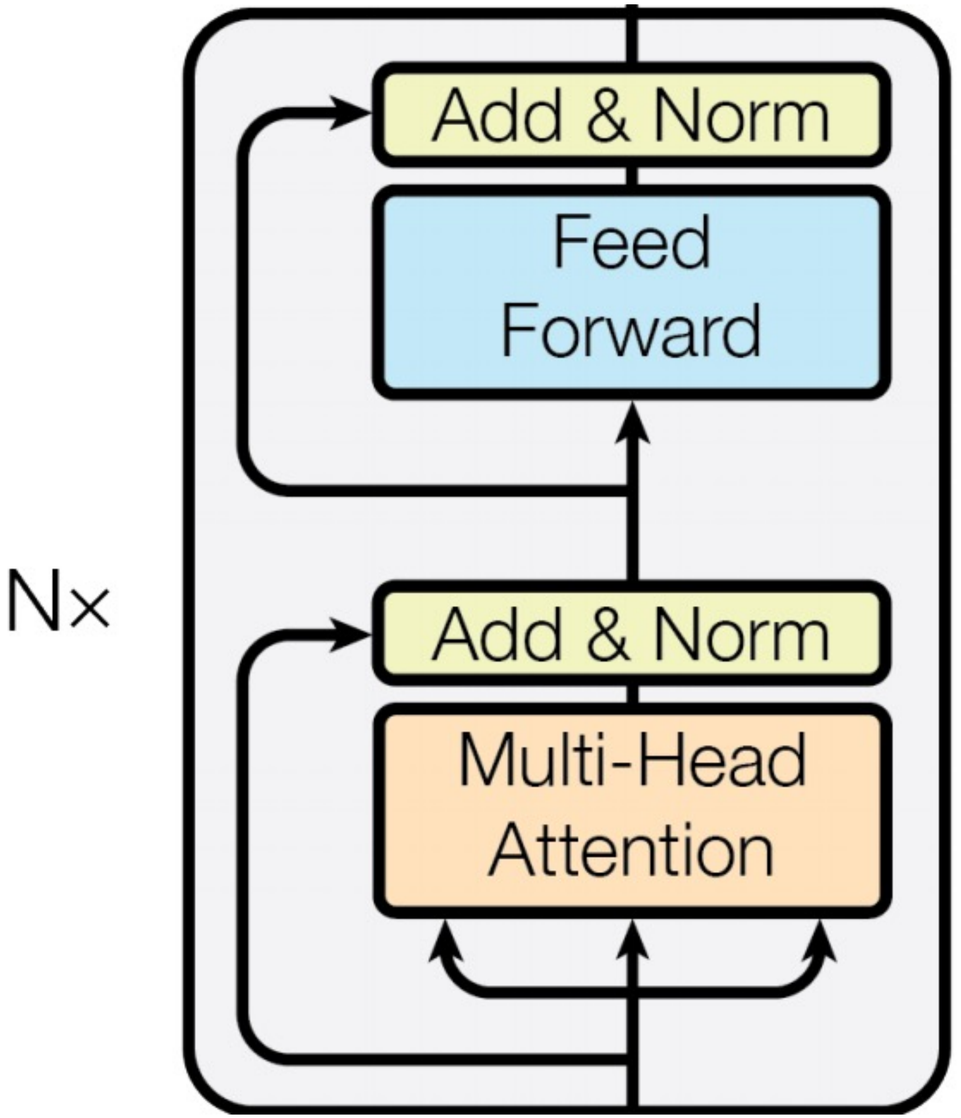
Multi-head attention

- 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



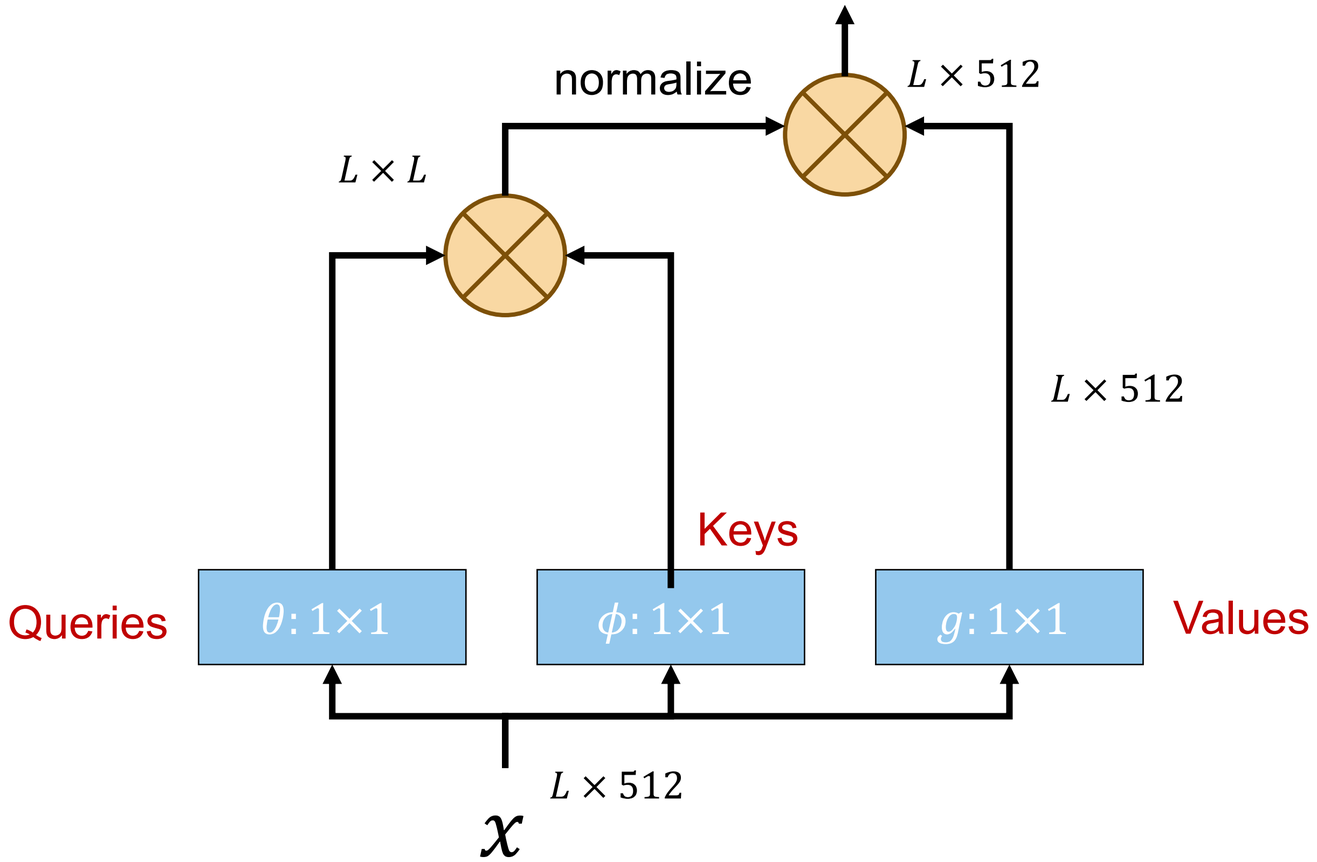
Transformer blocks

- 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

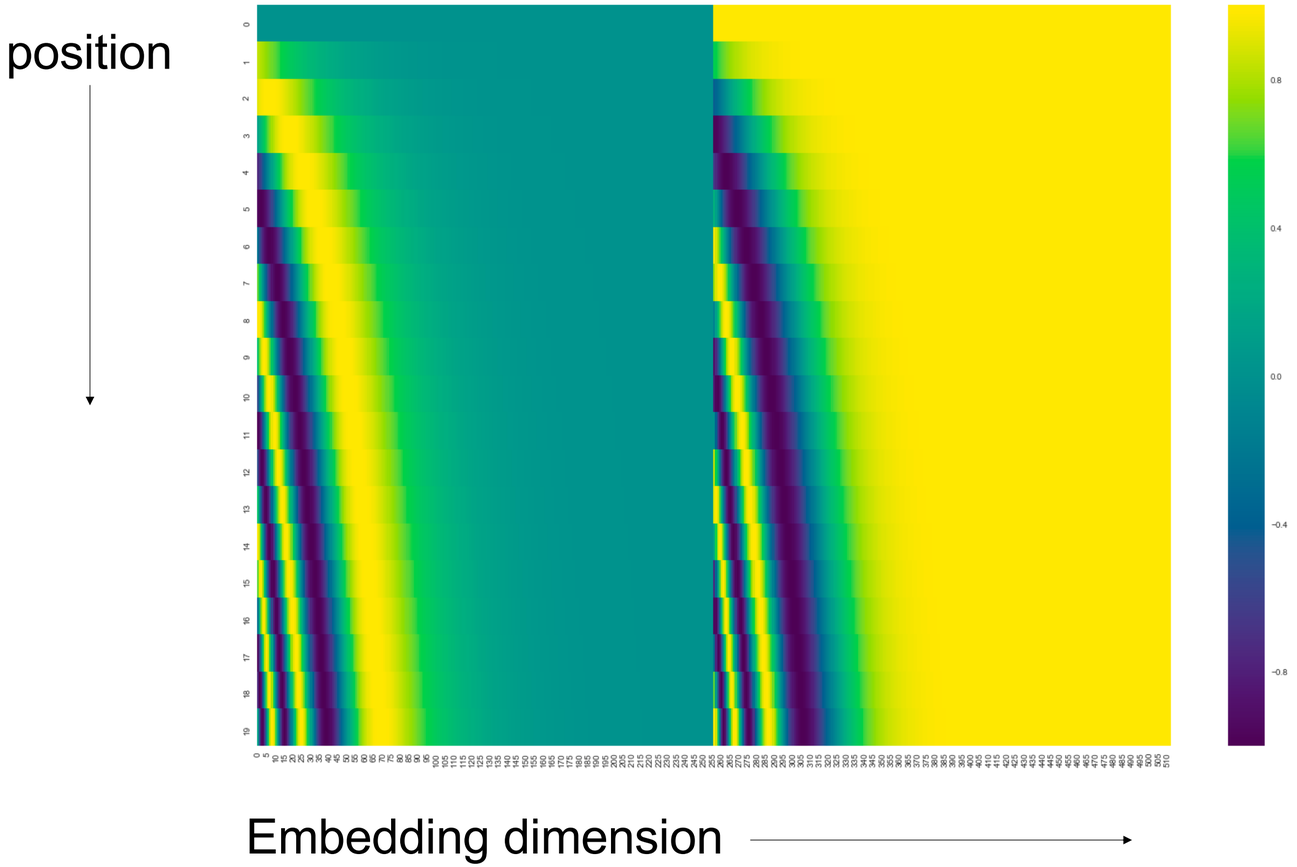
To give transformer information about ordering of tokens, add function of position (based on sines and cosines) to every input

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

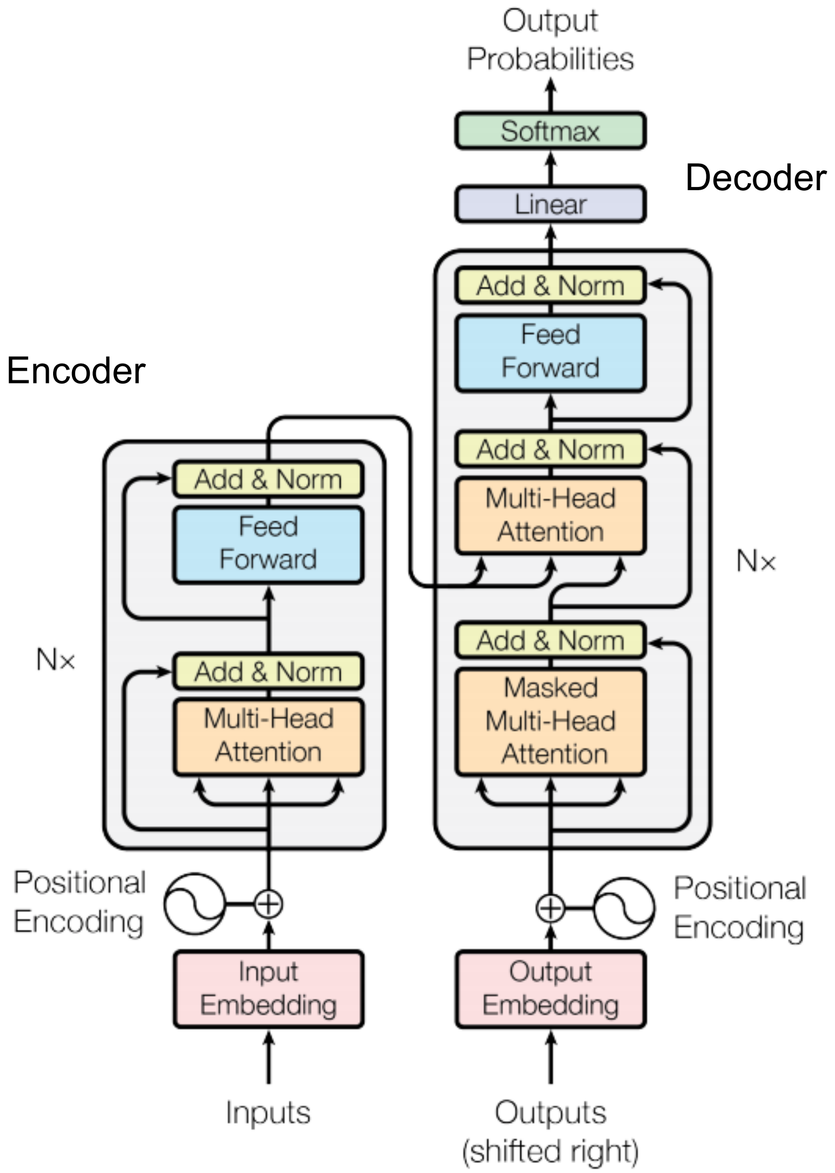
$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

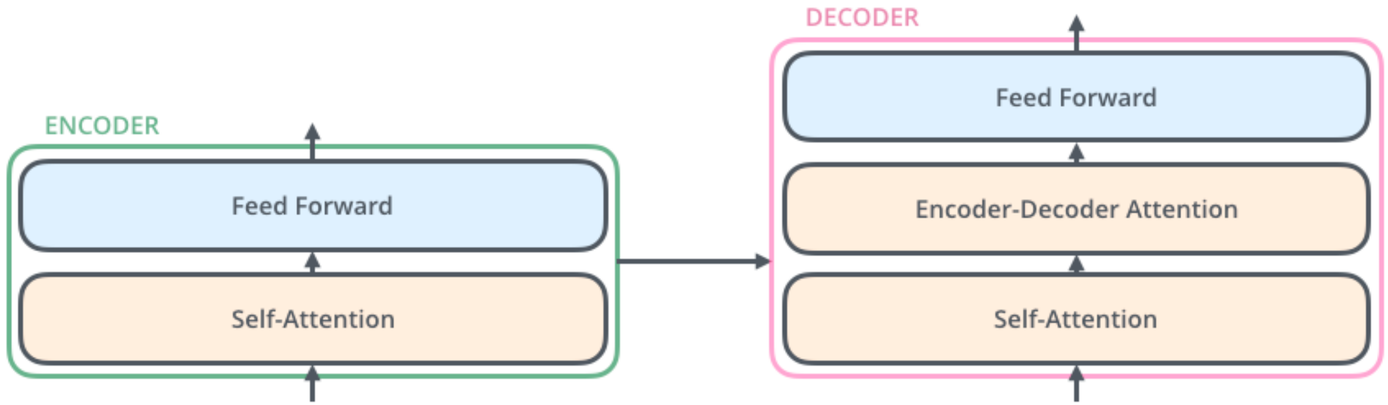
Positional encoding

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



Transformer architecture: Zooming back



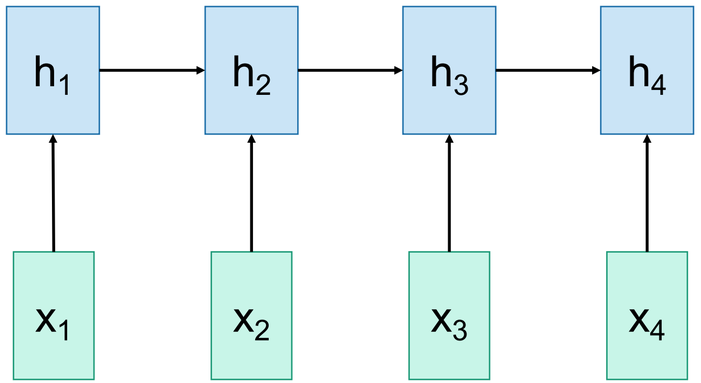


A. Vaswani et al., Attention is all you need, NeurIPS 2017


The
Law
will
never
be
perfect
,
but
its
application
should
be
just
-
this
is
what
we
are
missing
,
in
my
opinion
.
<EOS>
<pad>
The
Law
will
never
be
perfect
,
but
its
application
should
be
just
-
this
is
what
we
are
missing
,
in
my
opinion
.
<EOS>
<pad>

Different ways of processing sequences

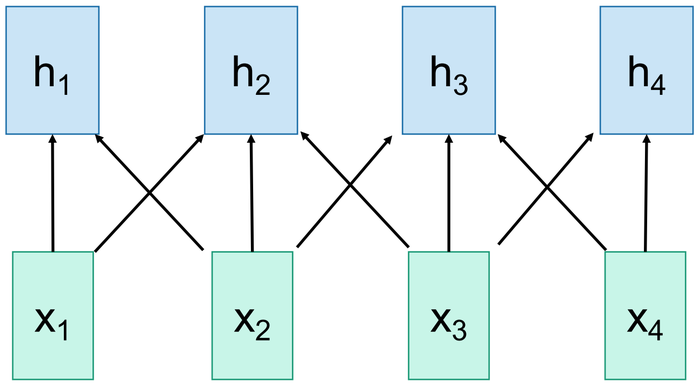
RNN



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

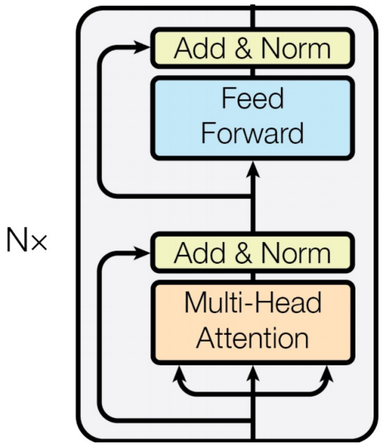
1D convolutional network



Works on **multidimensional grids**

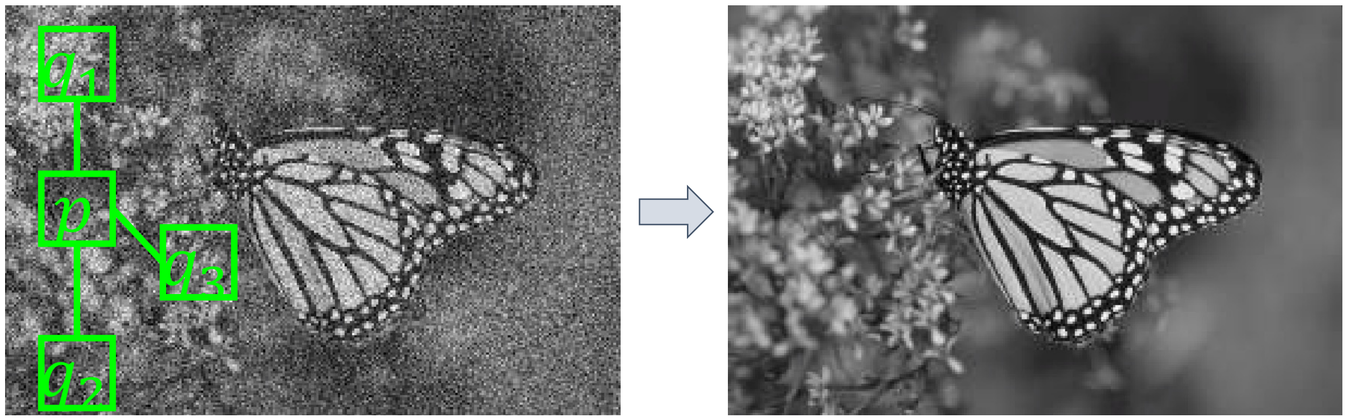
- Con: Bad at long sequences: Need to stack many conv layers for outputs to “see” the whole sequence
- Pro: Highly parallel: Each output can be computed in parallel

Transformer

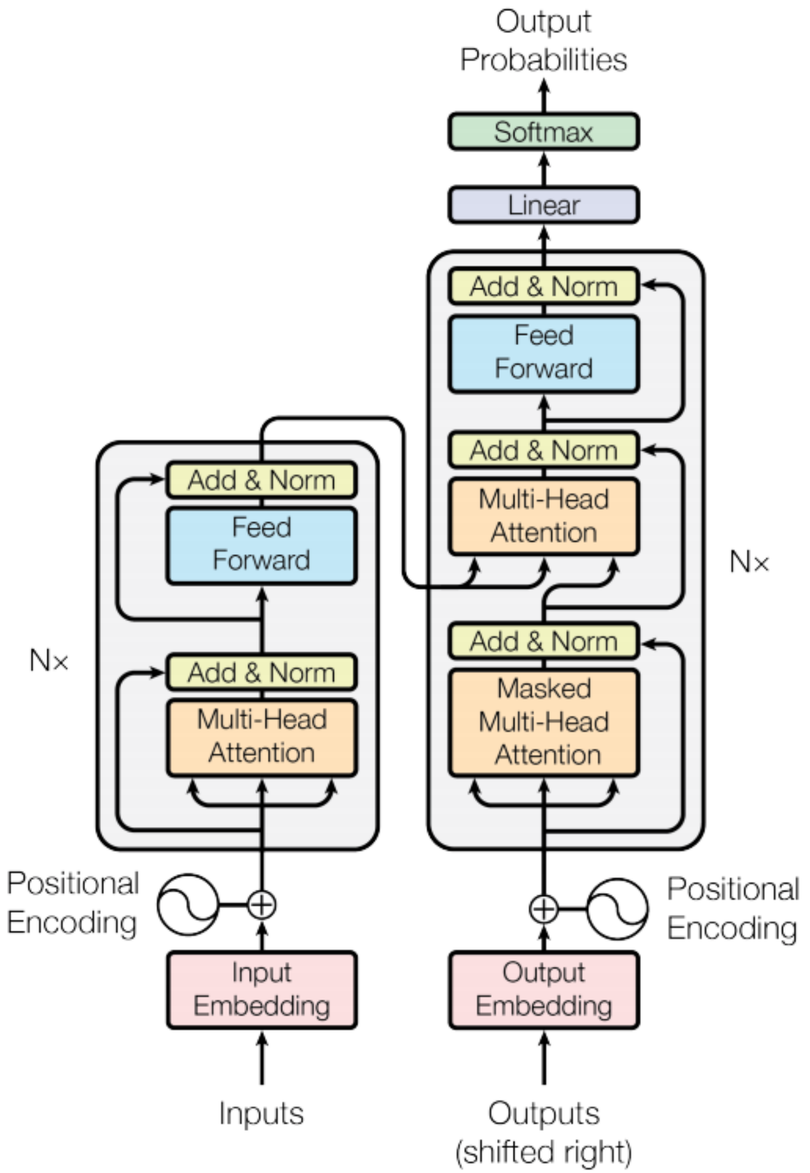


- Works on **sets of vectors**
- Pro: Good at long sequences: after one self-attention layer, each output “sees” all inputs!
- Pro: Highly parallel: Each output can be computed in parallel
- Con: Very memory-intensive

It is all Non-local Means



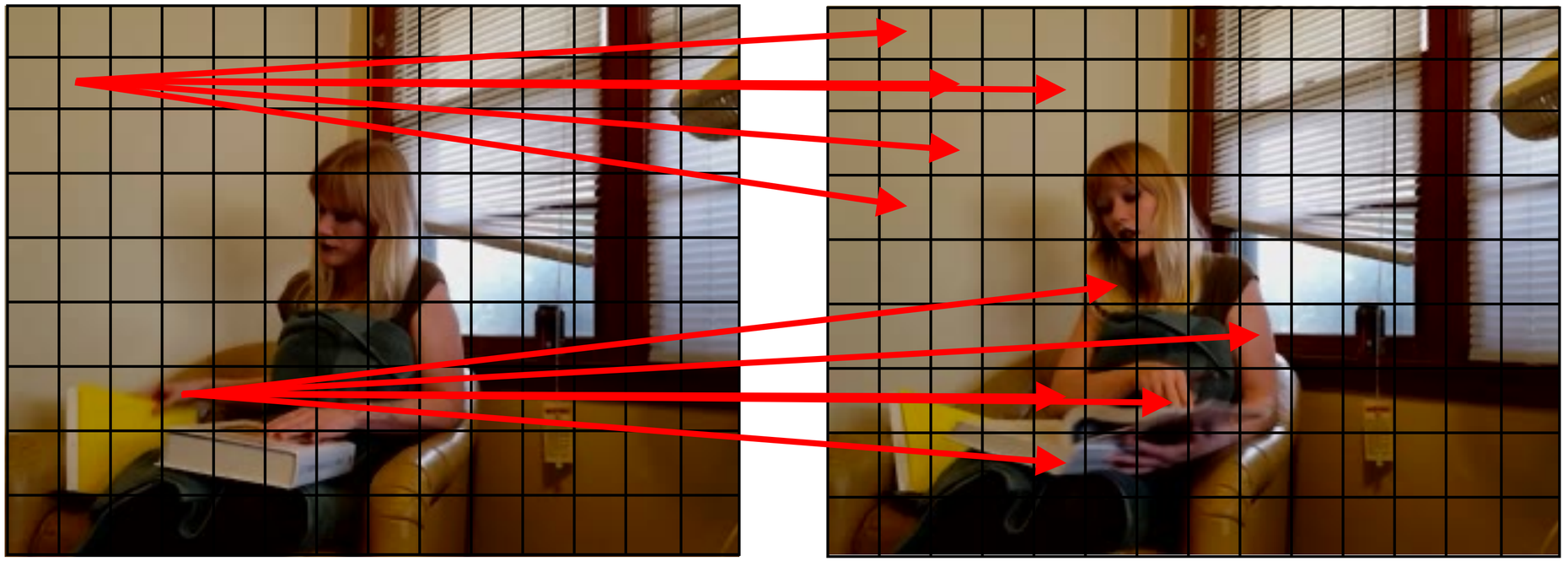
Buades et al., 2005.



Graph Neural Networks

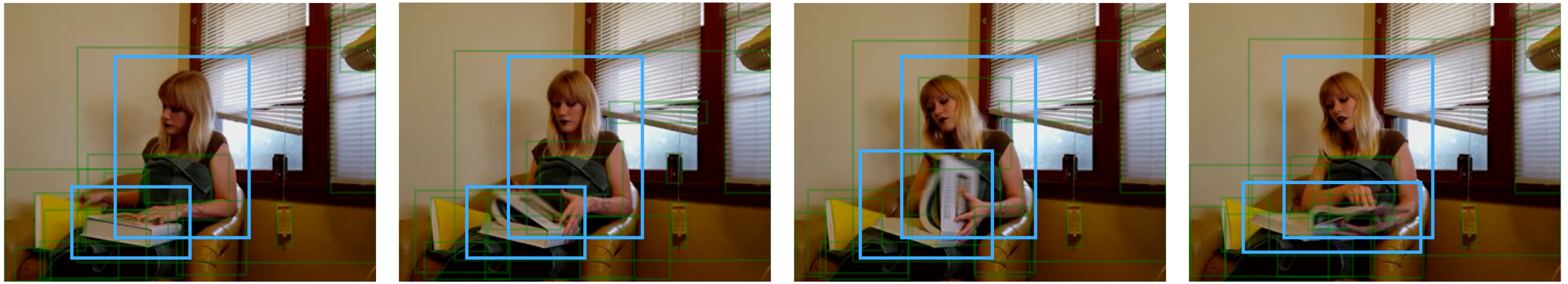
Opening A Book

Opening A Book



The Non-local / Self-Attention Block

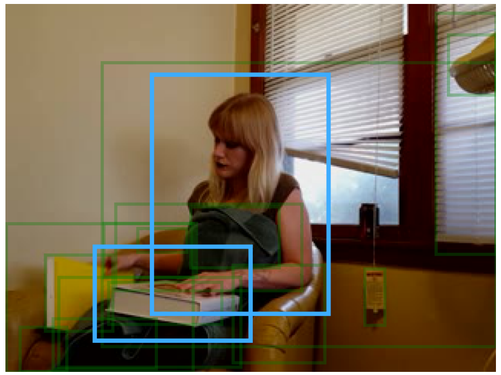
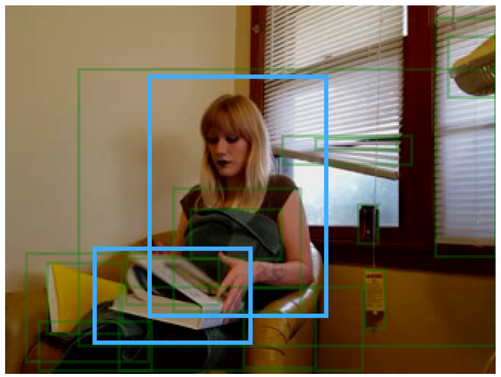
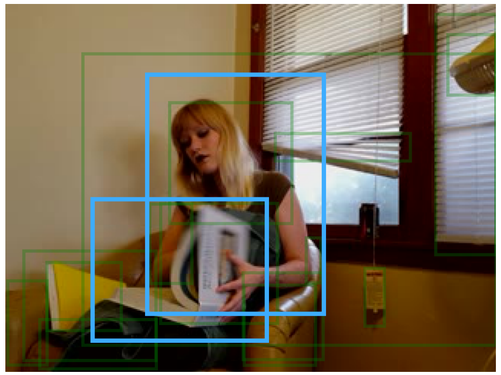
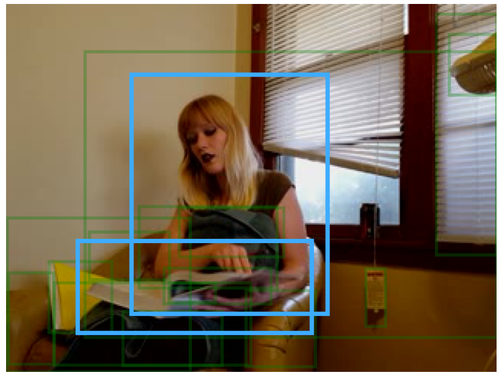
Opening A Book

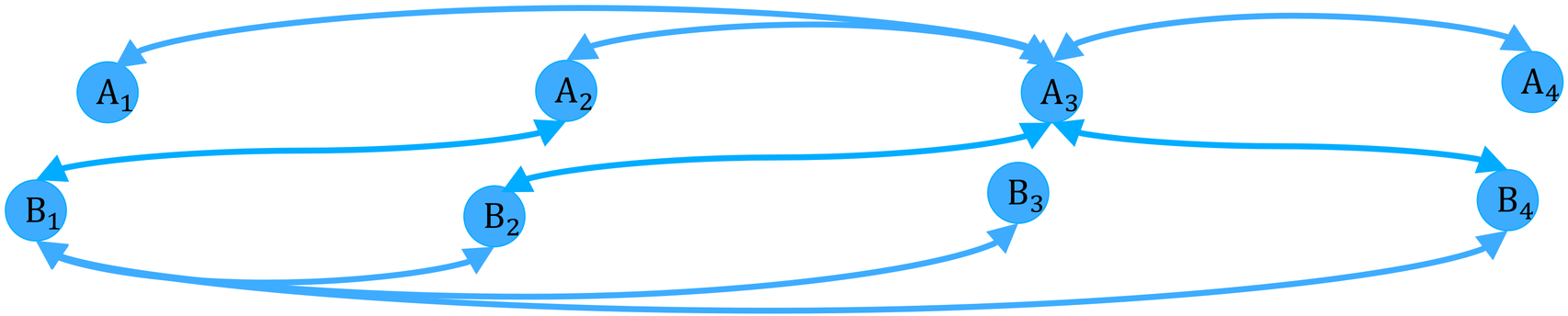


Object states changes over time

Human-object, object-object interactions

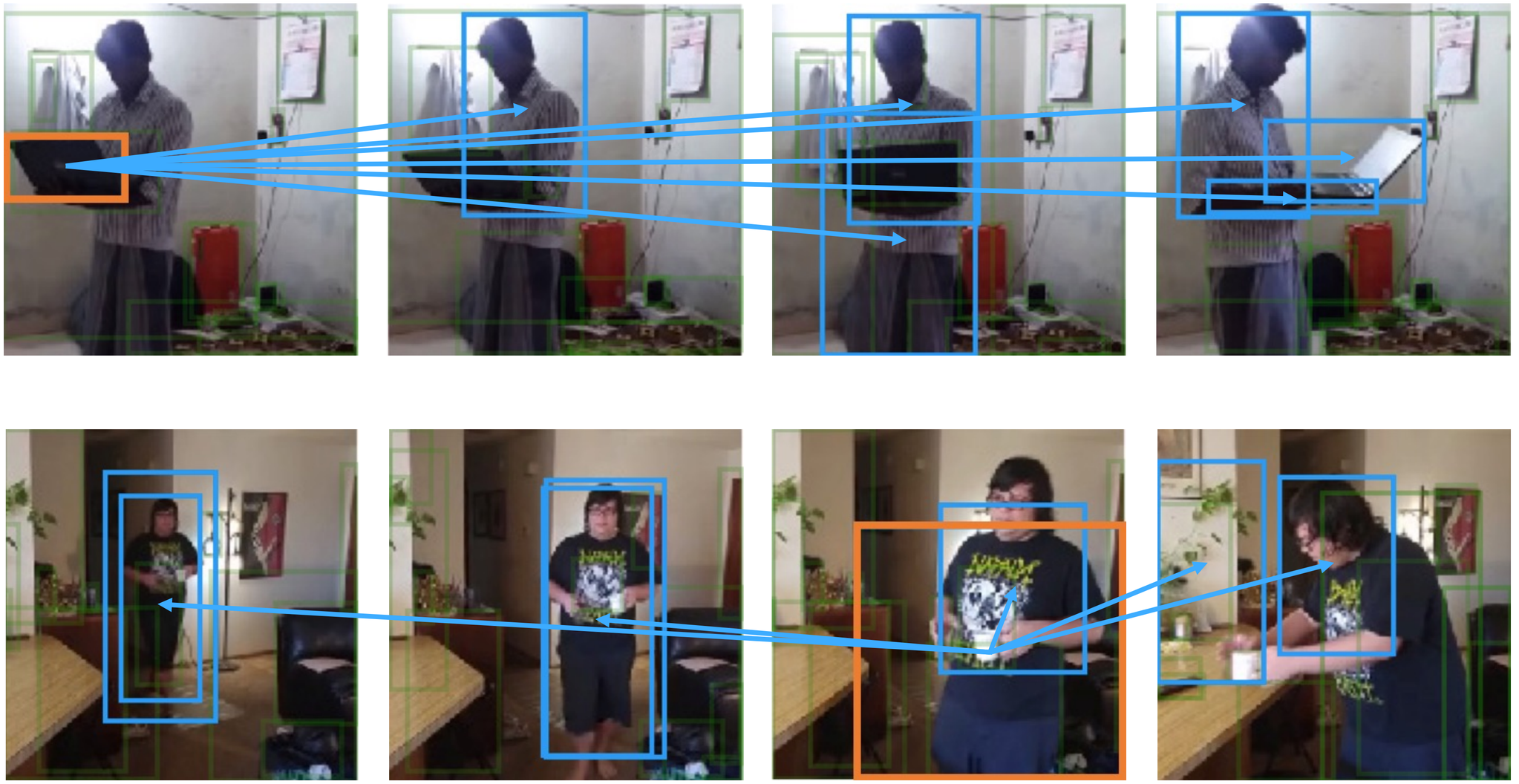
Opening A Book

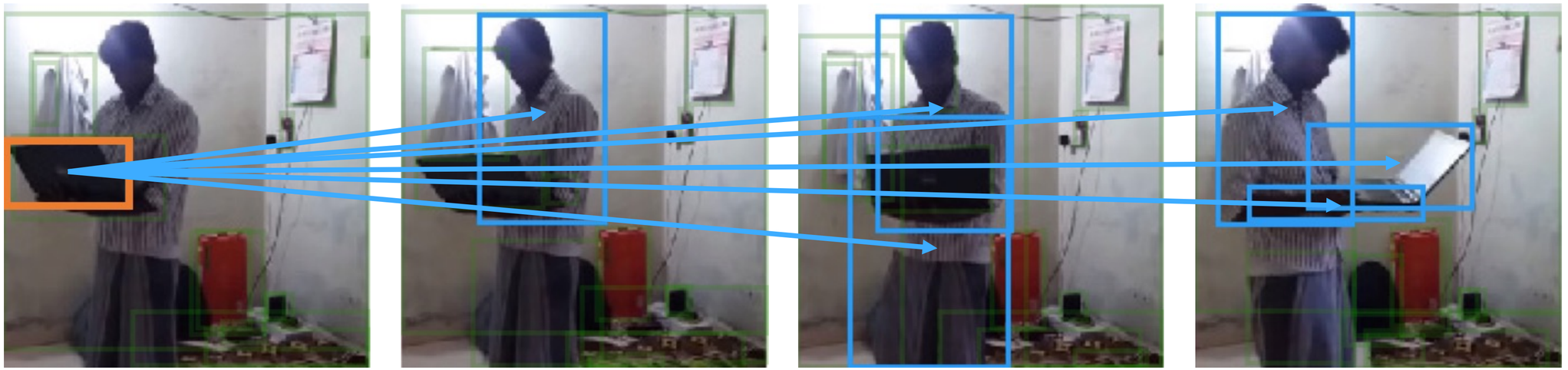


Highly Correlated

Relations between Regions



Relations between Regions



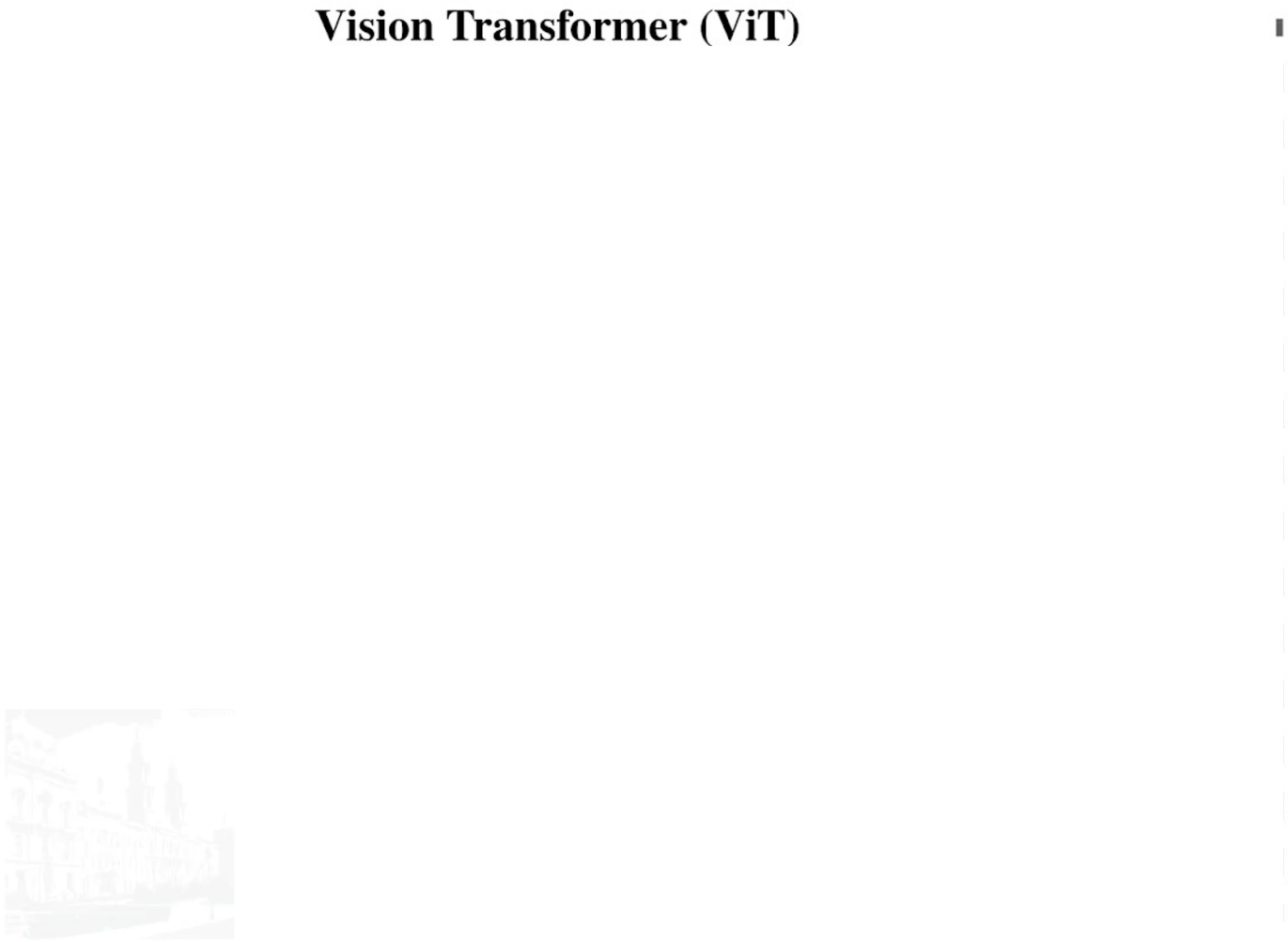
$$f(x_i, x_j) = \phi(x_i)^T \, \phi'(x_j)$$

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

Vision Transformer

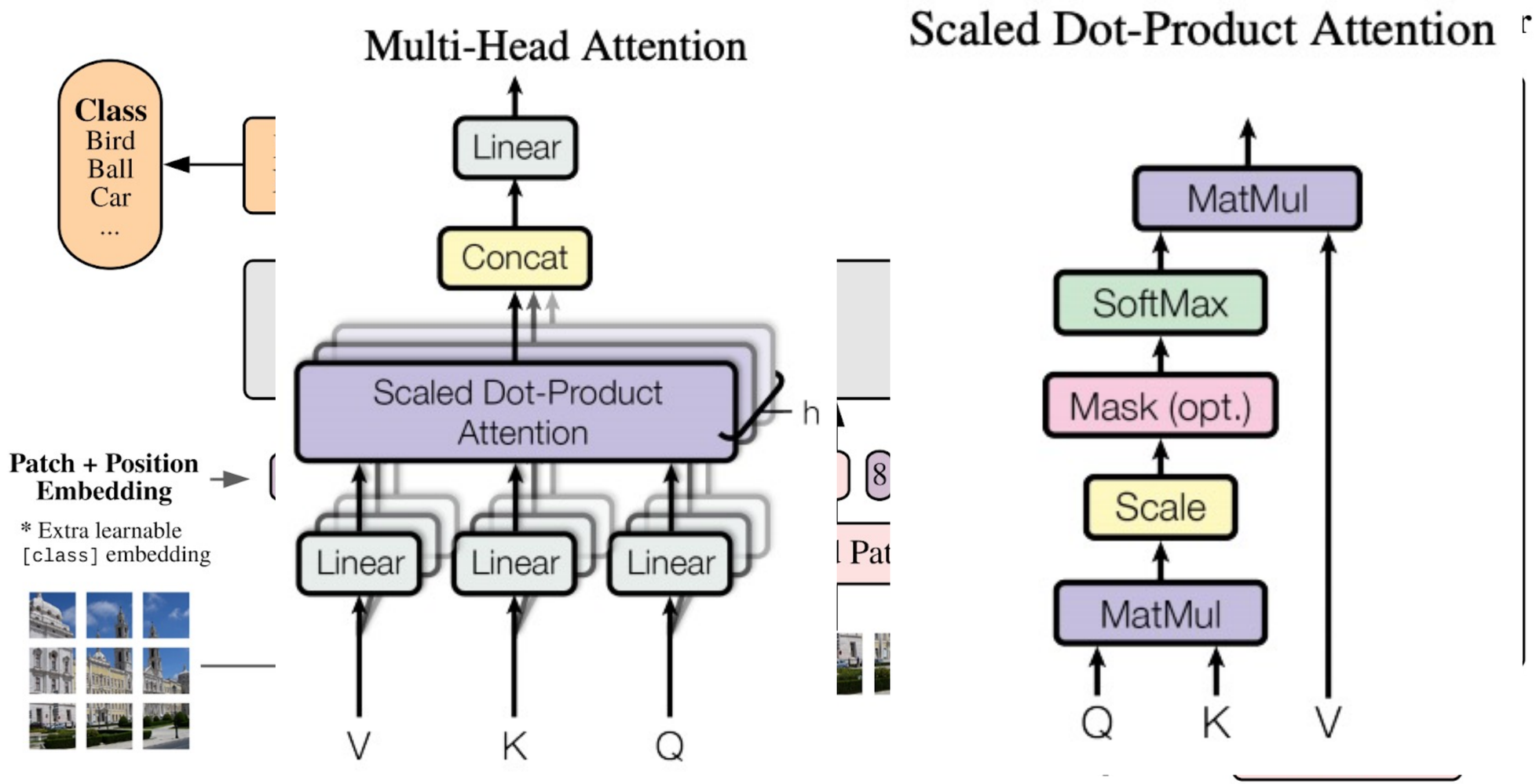
Xiaolong Wang

Vanilla ViT

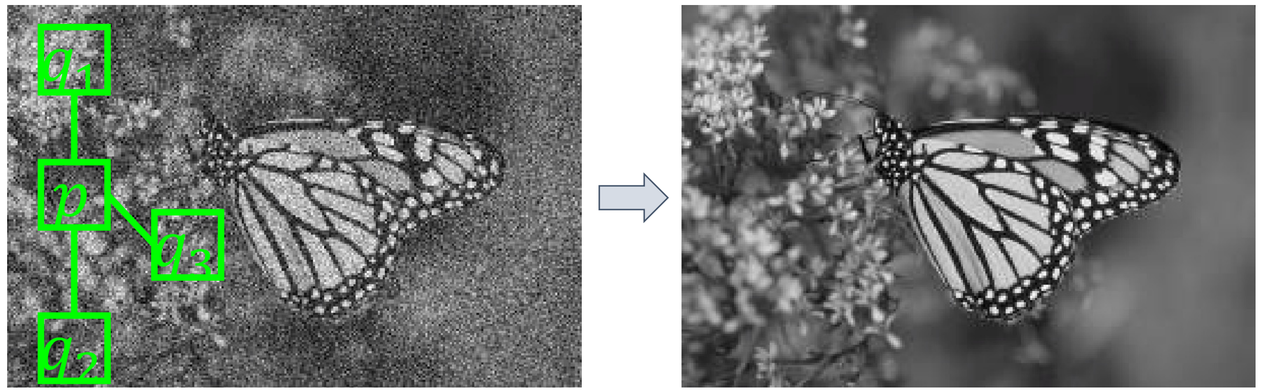


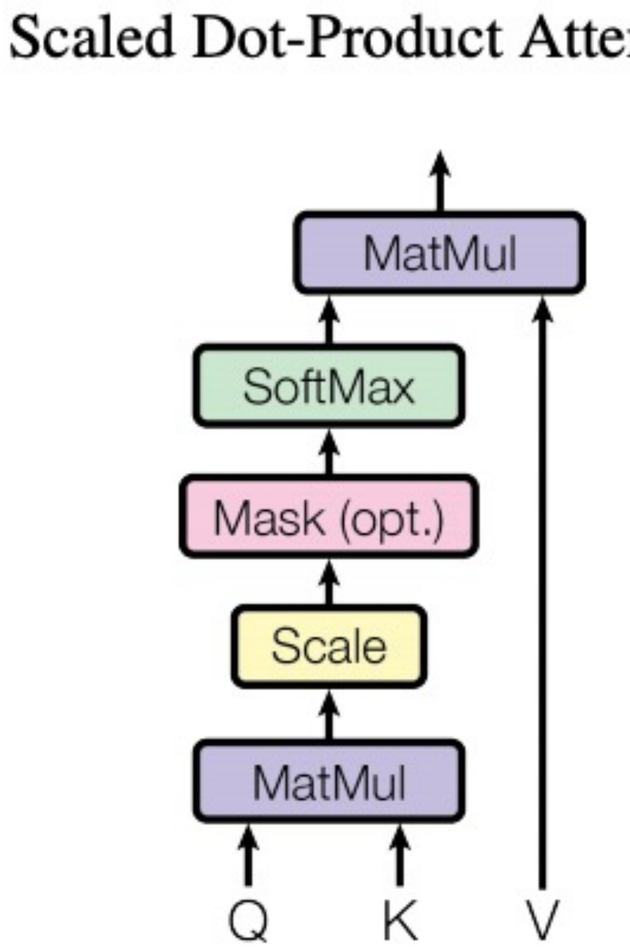
Dosovitskiy, Beyer, Kolesnikov, Weissenborn and Zhai et al. An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale . 2020

Vanilla ViT

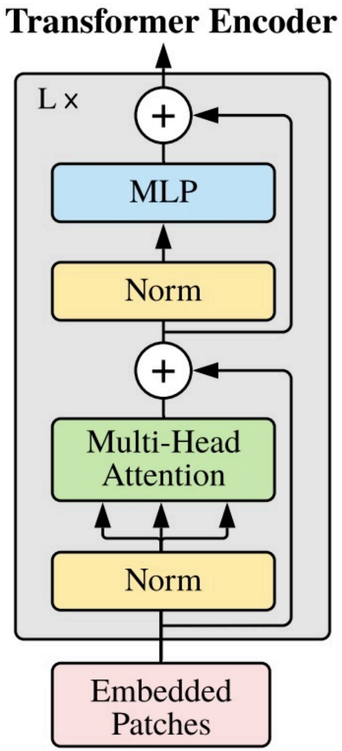

Class
Bird
Ball
Car
...
Patch + Position Embedding
* Extra learnable [class] embedding
Multi-Head Attention
Linear
Concat
Scaled Dot-Product Attention
h
Linear
Linear
Linear
V
K
Q
Scaled Dot-Product Attention
MatMul
SoftMax
Mask (opt.)
Scale
MatMul
Q
K
V

Vanilla ViT


g_1
p
g_3
g_2


Scaled Dot-Product Attention
MatMul
SoftMax
Mask (opt.)
Scale
MatMul
Q
K
V

Vanilla ViT



$$\mathbf{z}_0 = [\mathbf{x}_{\text{class}}; \mathbf{x}_p^1\mathbf{E}; \mathbf{x}_p^2\mathbf{E}; \cdots; \mathbf{x}_p^N\mathbf{E}] + \mathbf{E}_{pos}, \qquad \mathbf{E} \in \mathbb{R}^{(P^2 \cdot C) \times D}, \mathbf{E}_{pos} \in \mathbb{R}^{(N+1) \times D} \tag{1}$$

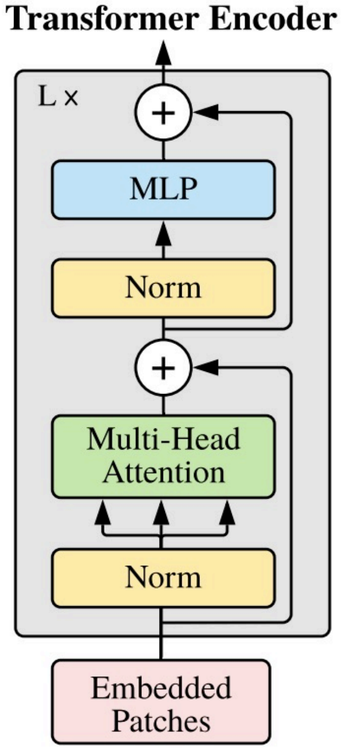
$$\mathbf{z}'_\ell = \text{MSA}(\text{LN}(\mathbf{z}_{\ell-1})) + \mathbf{z}_{\ell-1}, \qquad \ell = 1 \ldots L \tag{2}$$

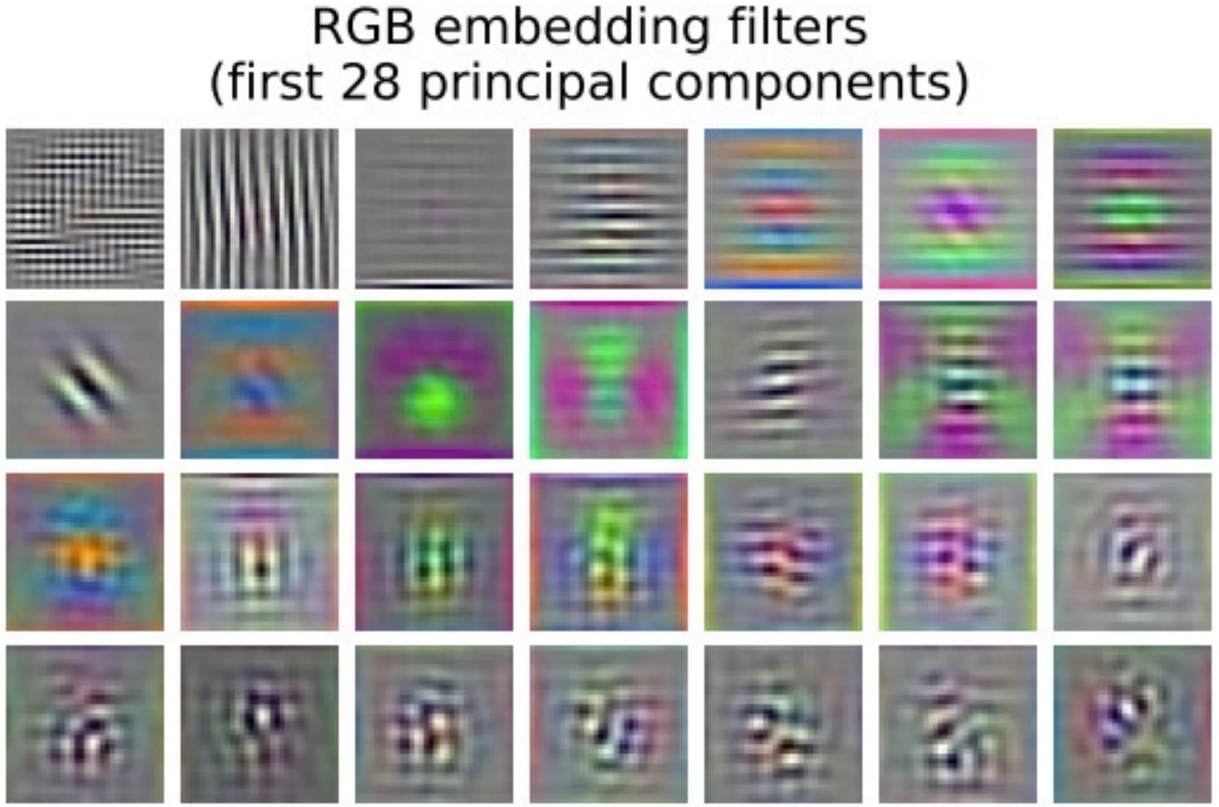
$$\mathbf{z}_\ell = \text{MLP}(\text{LN}(\mathbf{z}'_\ell)) + \mathbf{z}'_\ell, \qquad \ell = 1 \ldots L \tag{3}$$

$$\mathbf{y} = \text{LN}(\mathbf{z}_L^0) \tag{4}$$

Vanilla ViT

- ViT-L / 32 model first layer, it means the patch has 32 x 32 pixels





Model	Layers	Hidden size D	MLP size	Heads	Params
ViT-Base	12	768	3072	12	86M
ViT-Large	24	1024	4096	16	307M
ViT-Huge	32	1280	5120	16	632M

Vanilla ViT

- Previous CNN is tiny compared with ViT models
- CNN is much faster

Network	#param.	image size	throughput (image/s)	ImNet top-1
Convnets				
ResNet-18 [21]	12M	224^2	4458.4	69.8
ResNet-50 [21]	25M	224^2	1226.1	76.2
ResNet-101 [21]	45M	224^2	753.6	77.4
ResNet-152 [21]	60M	224^2	526.4	78.3
RegNetY-4GF [40]⋆	21M	224^2	1156.7	80.0
RegNetY-8GF [40]⋆	39M	224^2	591.6	81.7
RegNetY-16GF [40]⋆	84M	224^2	334.7	82.9
ViT-B/16 [15]	86M	384^2	85.9	77.9
ViT-L/16 [15]	307M	384^2	27.3	76.5
DeiT-Ti	5M	224^2	2536.5	72.2
DeiT-S	22M	224^2	940.4	79.8
DeiT-B	86M	224^2	292.3	81.8
DeiT-B↑384	86M	384^2	85.9	83.1

DeiT: Touvron and Cord et al. 2020

Vanilla ViT

- Small and Base size model could be improved with strong data augmentation and regularization (DeiT)
- More data helps ViT (ImageNet-22K, JFT-300M)

1.3M Images

(a) Regular ImageNet-1K trained models

method	image size	#param.	FLOPs	throughput (image / s)	ImageNet top-1 acc.
ViT-B/16 [19]	384^2	86M	55.4G	85.9	77.9
ViT-L/16 [19]	384^2	307M	190.7G	27.3	76.5
DeiT-S [60]	224^2	22M	4.6G	940.4	79.8
DeiT-B [60]	224^2	86M	17.5G	292.3	81.8
DeiT-B [60]	384^2	86M	55.4G	85.9	83.1

(b) ImageNet-22K pre-trained models 14M Images

method	image size	#param.	FLOPs	throughput (image / s)	ImageNet top-1 acc.
ViT-B/16 [19]	384^2	86M	55.4G	85.9	84.0
ViT-L/16 [19]	384^2	307M	190.7G	27.3	85.2

(c) JFT-300M pre-trained models 300M Images

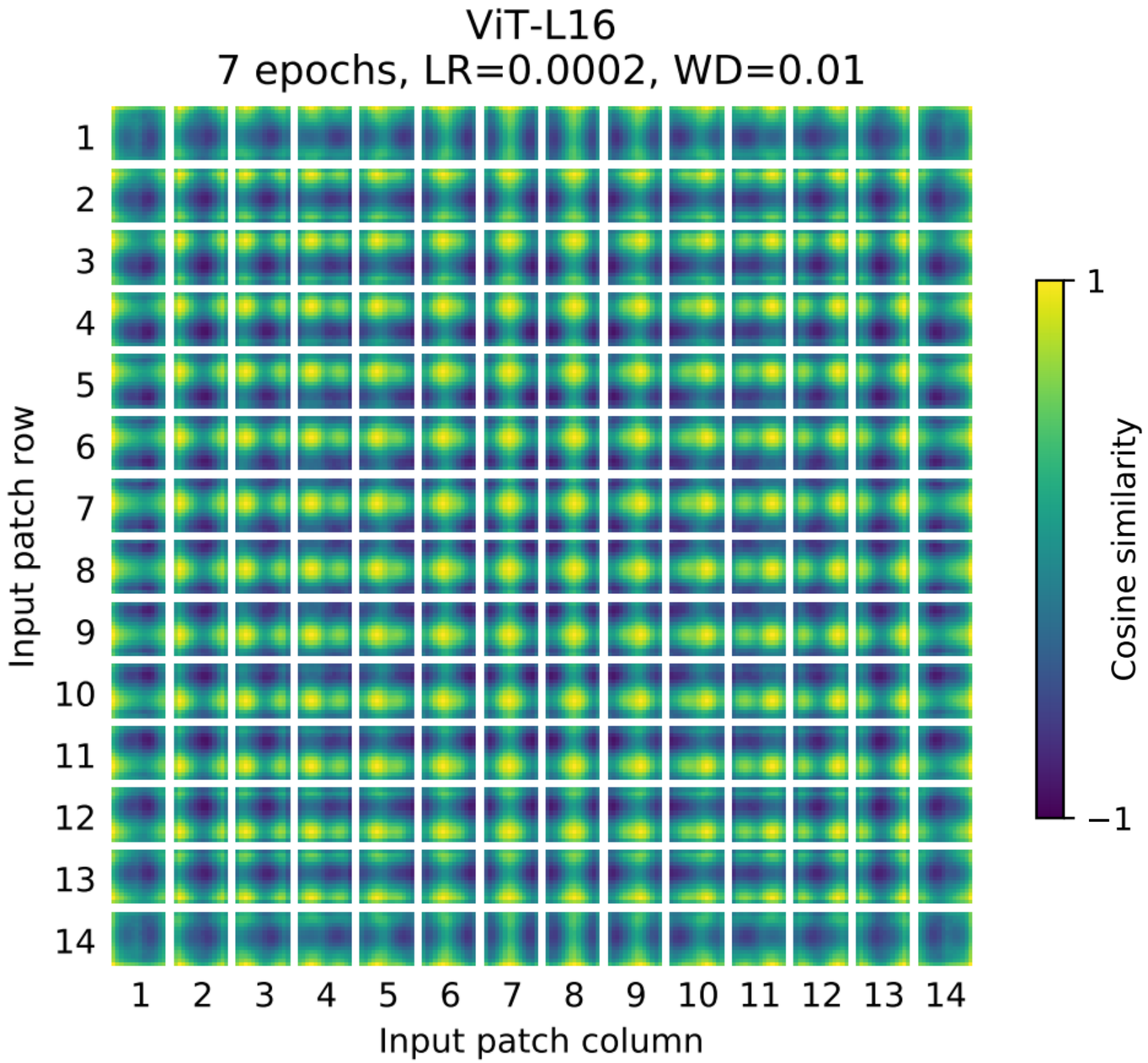
method	image size	#param.	FLOPs	throughput (image / s)	ImageNet top-1 acc.
ViT-B/16 [19]	384^2	86M	55.4G	85.9	84.2
ViT-L/16 [19]	384^2	307M	190.7G	27.3	87.1
ViT-H/14 [19]	384^2	307M	190.7G	27.3	88.1

DeiT: Touvron and Cord et al. 2020

Vanilla ViT

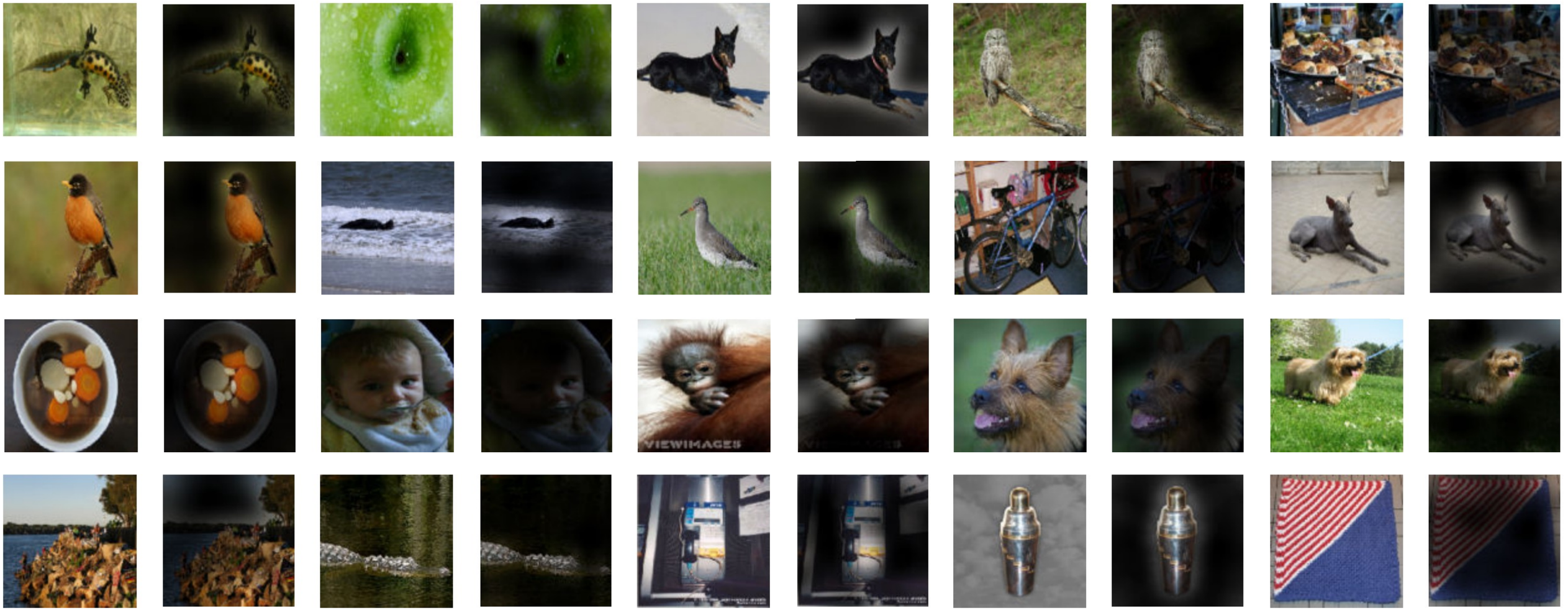
- ViT learns intuitive local structures
- Closer patches tend to have more similarity of position embeddings

Each patch shows the position embedding cosine similarity between the patch at this location and all other patches



ViT: Dosovitskiy, Beyer, Kolesnikov, Weissenborn and Zhai et al. 2020

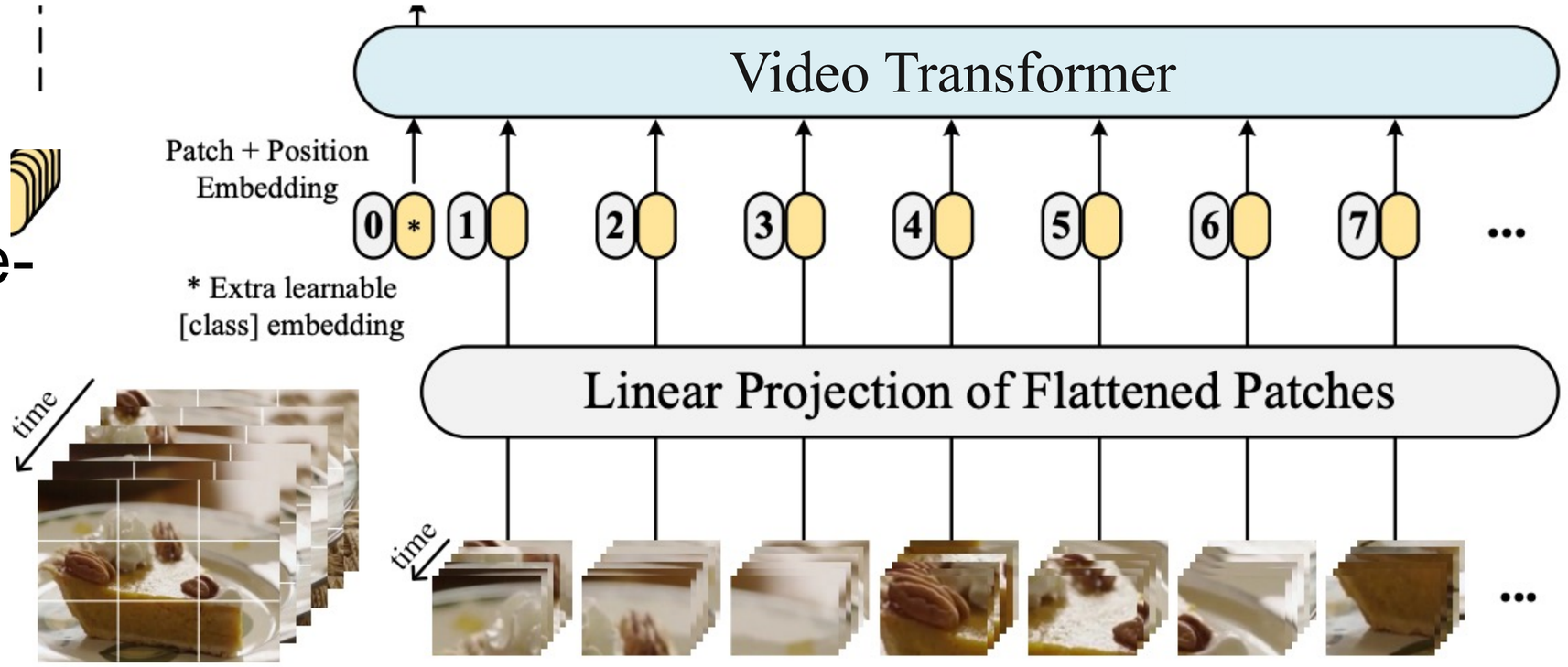
Vanilla ViT



Transformer in Videos

TimeSformer

- Share similar structure as ViT
- Video clip as a sequence of frame-level patches (16x16)



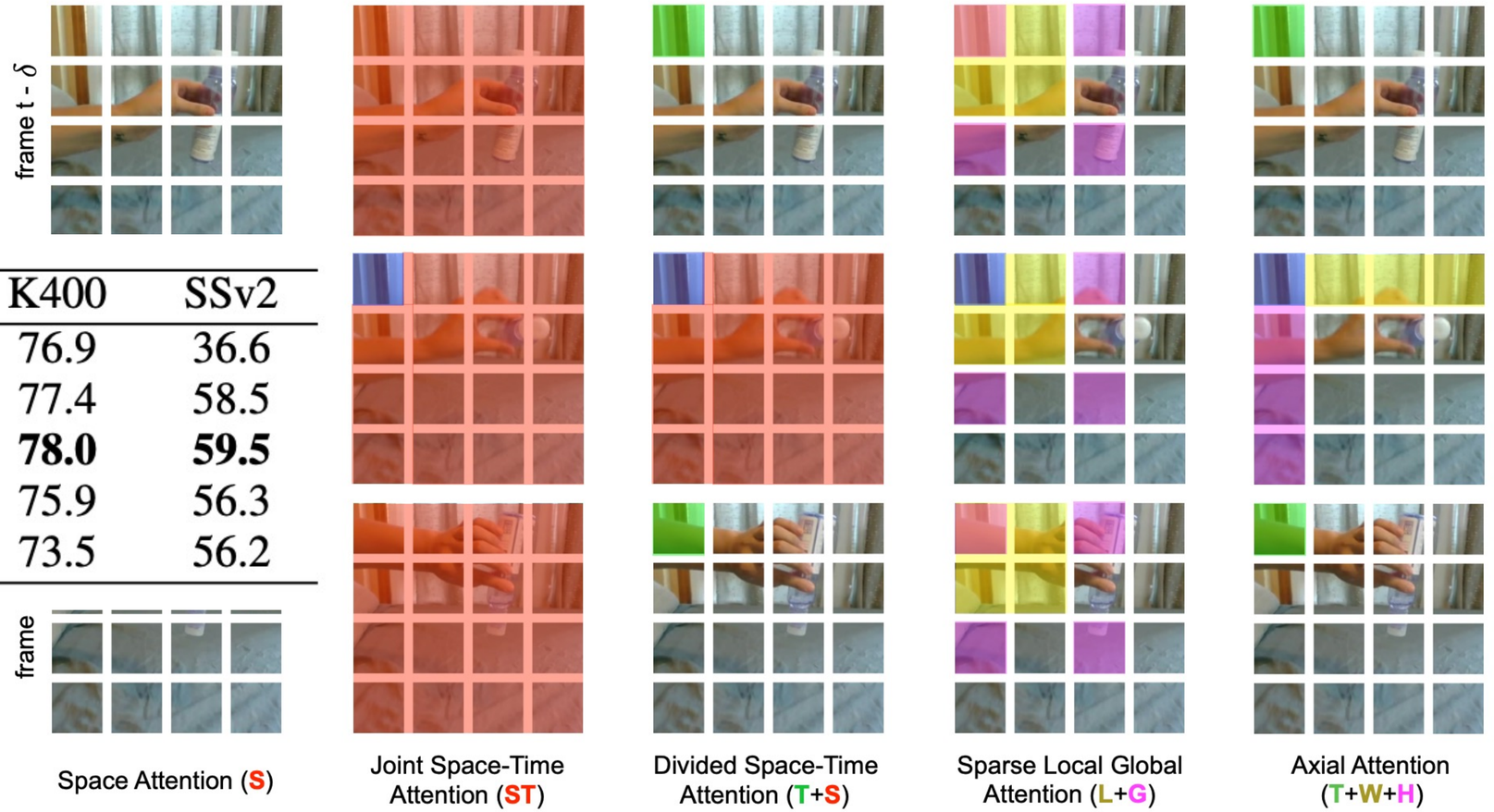
TimeSformer: Bertasius et al. 2021

Transformer in Videos

TimeSformer

- How to model temporal information?

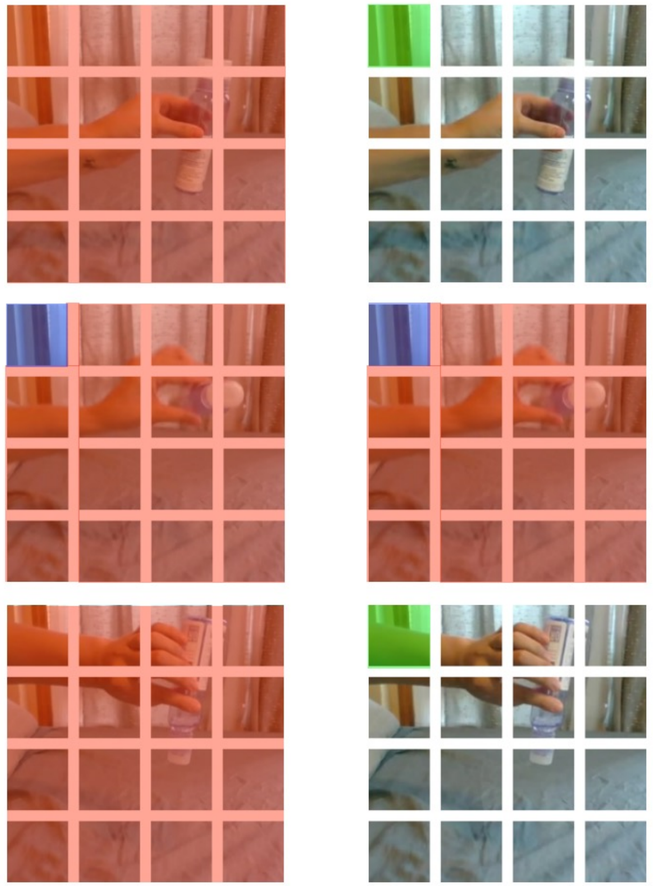
Attention	Params	K400	SSv2
Space	85.9M	76.9	36.6
Joint Space-Time	85.9M	77.4	58.5
Divided Space-Time	121.4M	**78.0**	**59.5**
Sparse Local Global	121.4M	75.9	56.3
Axial	156.8M	73.5	56.2



TimeSformer: Bertasius et al. 2021

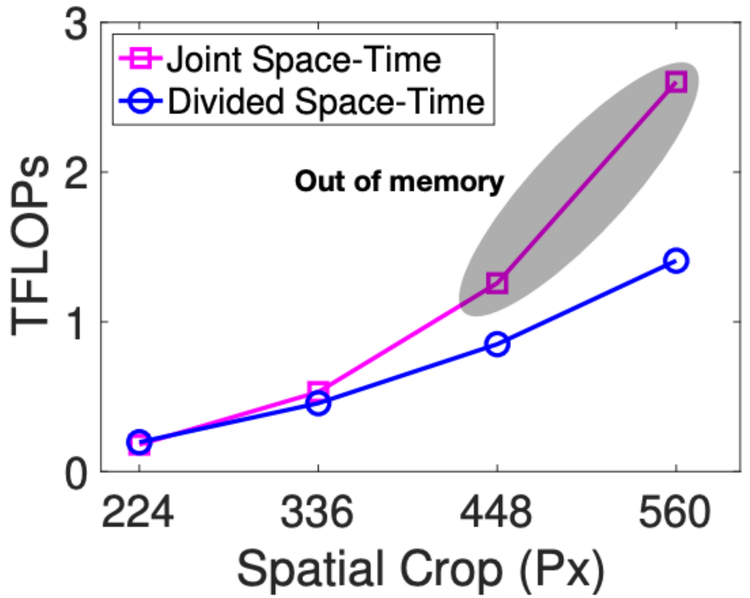
Transformer in Videos

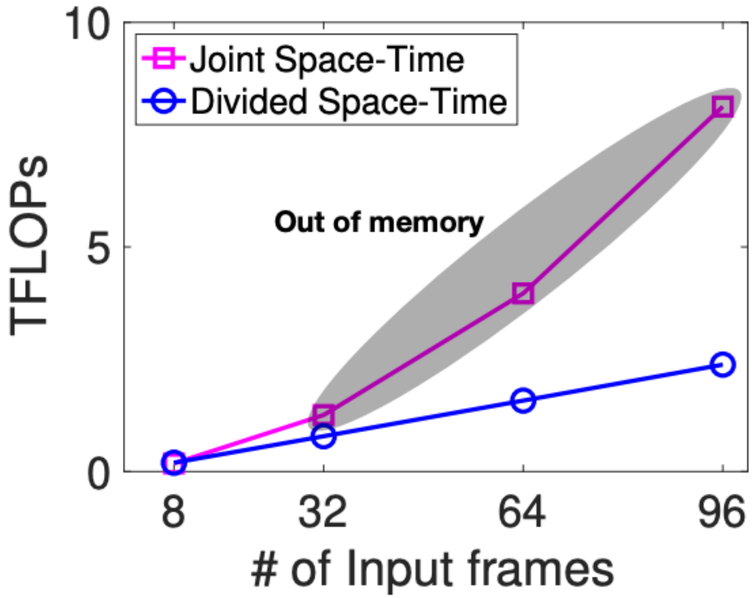
TimeSformer



Joint Space-Time Attention (**ST**)

Divided Space-Time Attention (**T**+**S**)

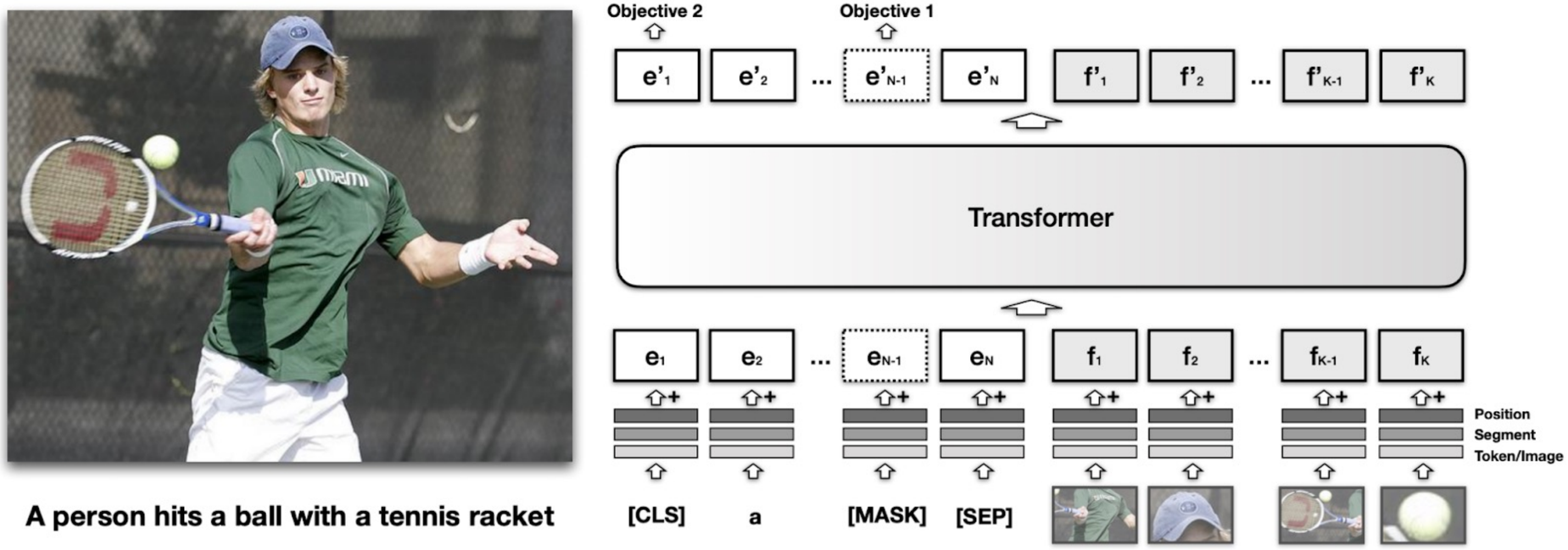




Transformer for Multi-modality

Image-Text

- Image patches are generated by pre-trained object detector
- Mask language modeling

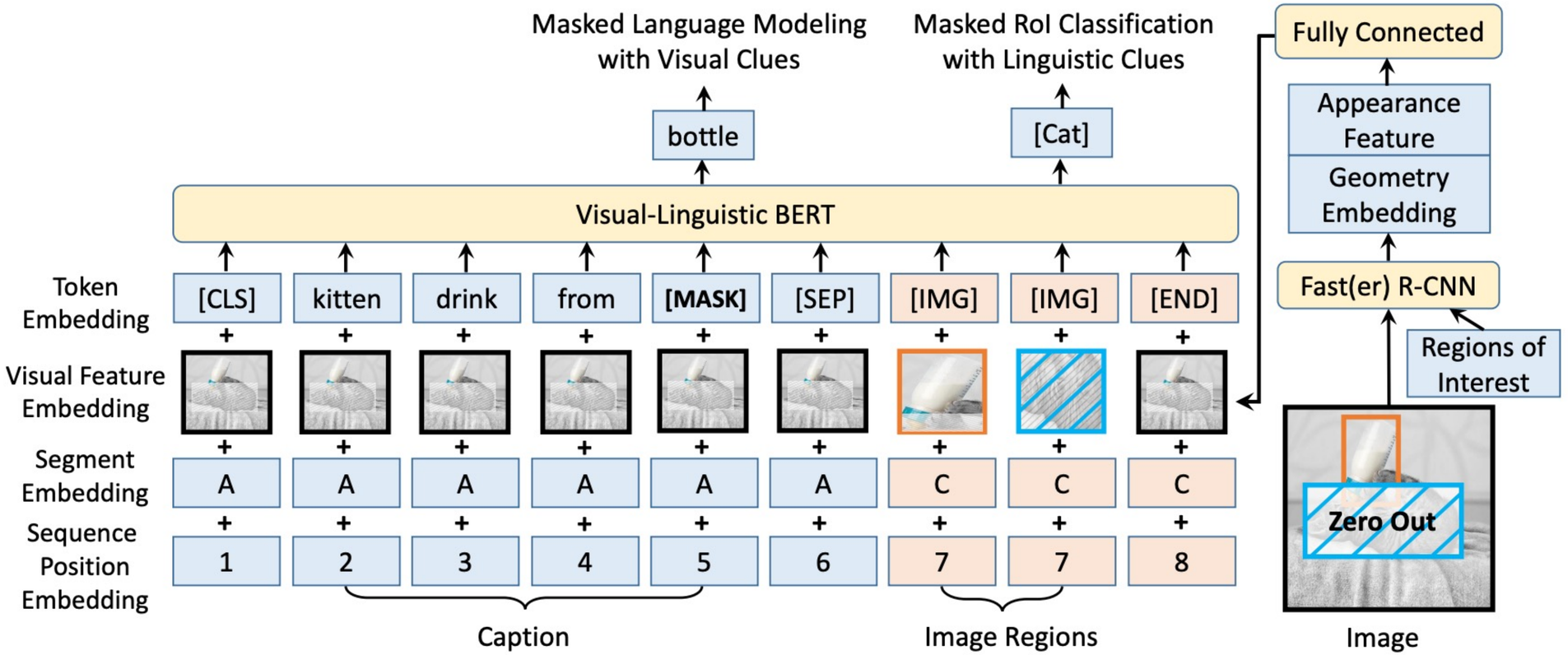


Visual-BERT: Li et al. 2019

Transformer for Multi-modality

Image-Text

- Extend with masked RoI classification

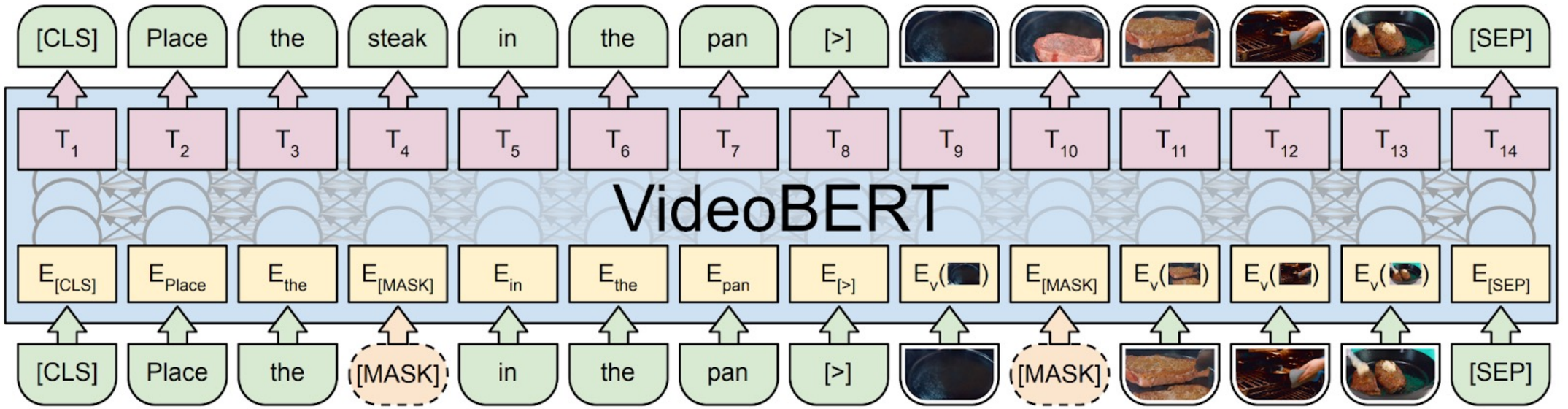


VL-BERT: Su et al. 2019

Transformer for Multi-modality

Video-Text

- Concatenate word sequence with video frame sequence
- Mask language modeling



VideoBERT: Sun et al. 2019