13. Vision Transformers

GEV6135 Deep Learning for Visual Recognition and Applications

Kibok Lee

Assistant Professor of

Applied Statistics / Statistics and Data Science

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연세대학교
YONSEI UNIVERSITY

Assignment 7

- Due **Wednesday 12/14, 11:59pm KST**
- PyTorch autograd and nn
  - 3 different abstraction levels
  - Residual networks

- Before submitting your work, we recommend you
  - Re-download clean files
  - Copy-paste your solution to clean py
  - Re-run clean ipynb only once
- If you feel difficult, consider to take **option 2**.

Notes on Assignment

A3/4 grading is almost done, we are doing fine adjustment

- Do not cheat!
  - We observed suspected behaviors even without running the plagiarism check
  - If you made plagiarism mistakenly and want to fix it, send an email to our TA; we will give 0 point for that assignment only
- We check if:
  - Your implementation is correct
  - Your hyperparameter tuning result is satisfactory
  - You don’t bother our TA with any unexpected behavior
    - You should run all cells
    - You should not import additional libraries / use prohibited functions
  - You don’t have to submit empty files; it actually bothers our TA

Outline

- Recurrent Neural Networks
- Attention and Transformers
- Vision Transformers

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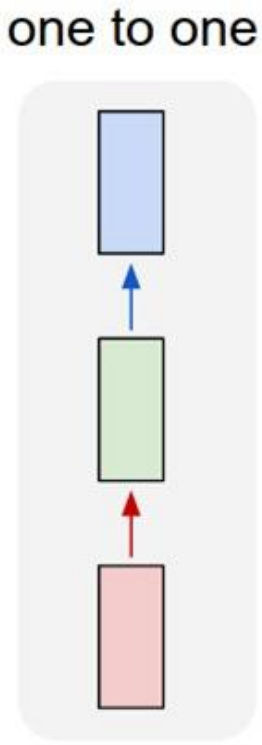
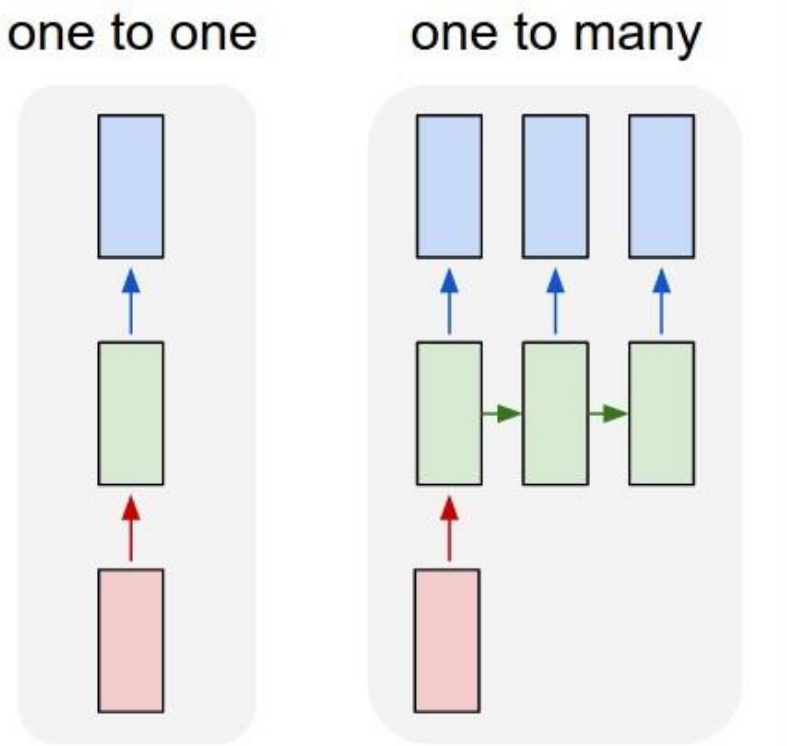
- Attention and Transformers
- Vision Transformers

So far: “Feedforward” Neural Networks



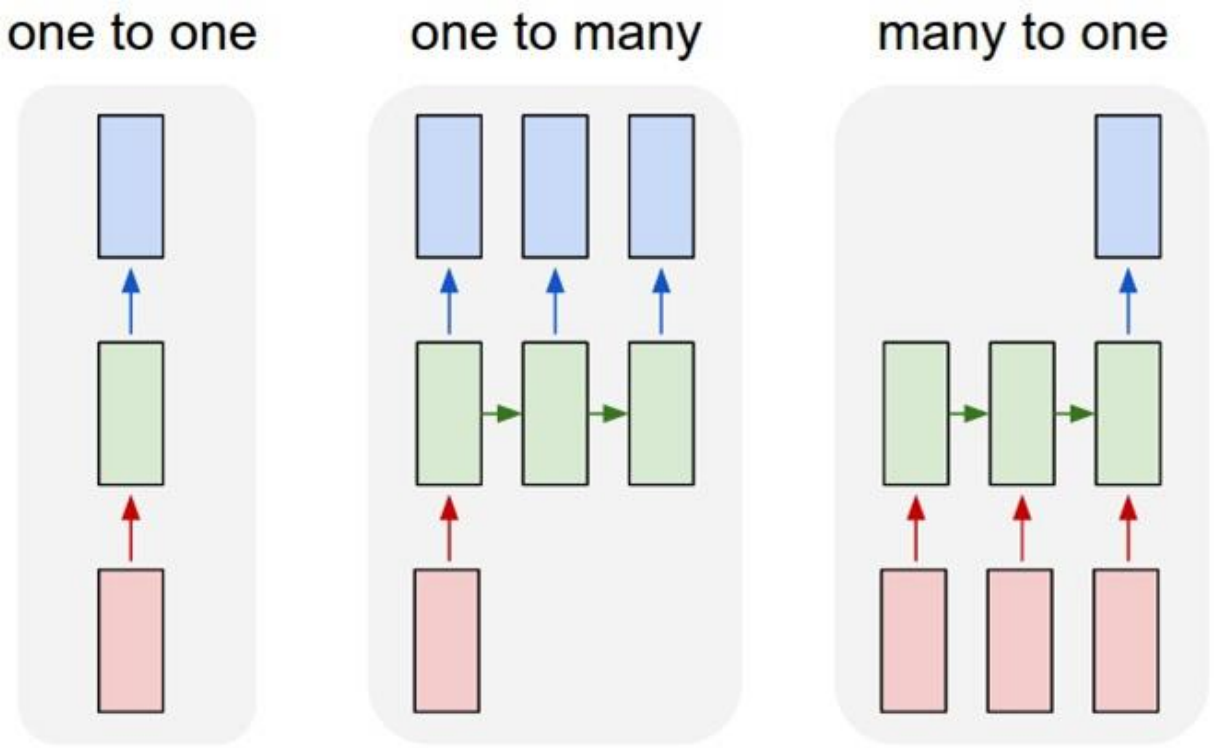
e.g., **Image classification**
Image -> Label

Recurrent Neural Networks: Process Sequences



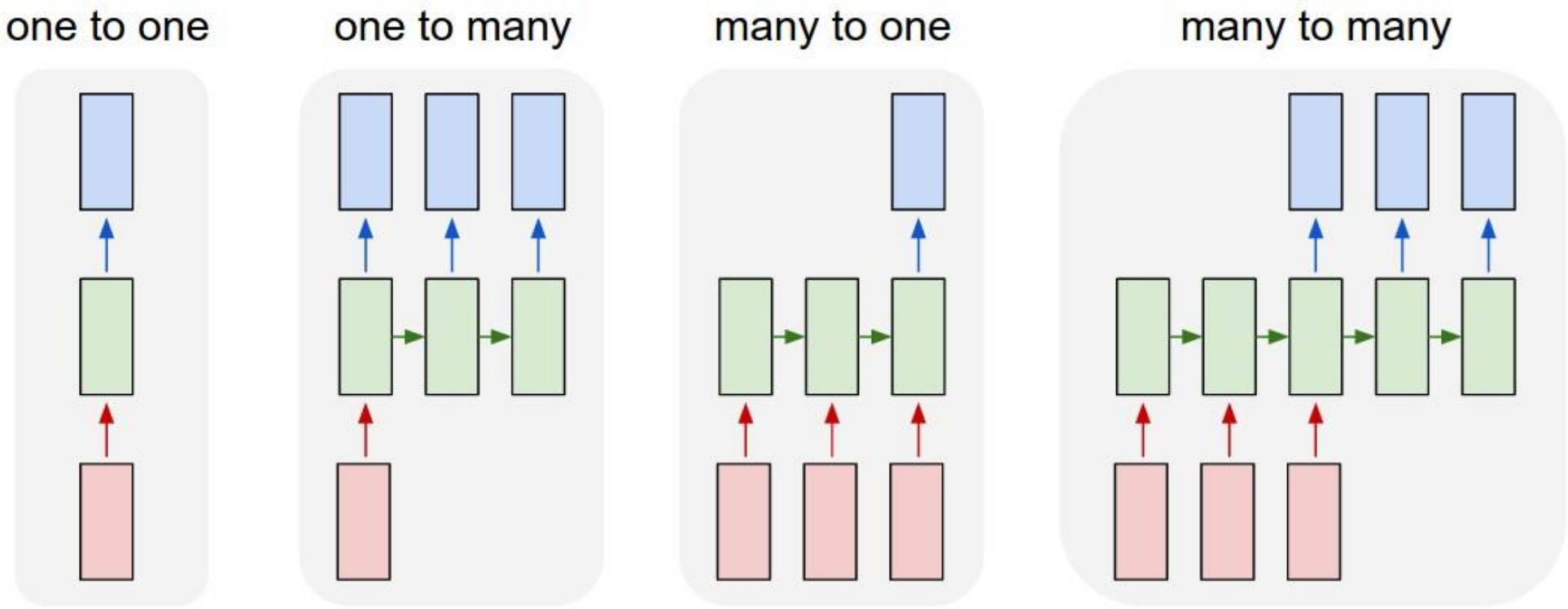
e.g., **Image Captioning**:
Image -> sequence of words

Recurrent Neural Networks: Process Sequences



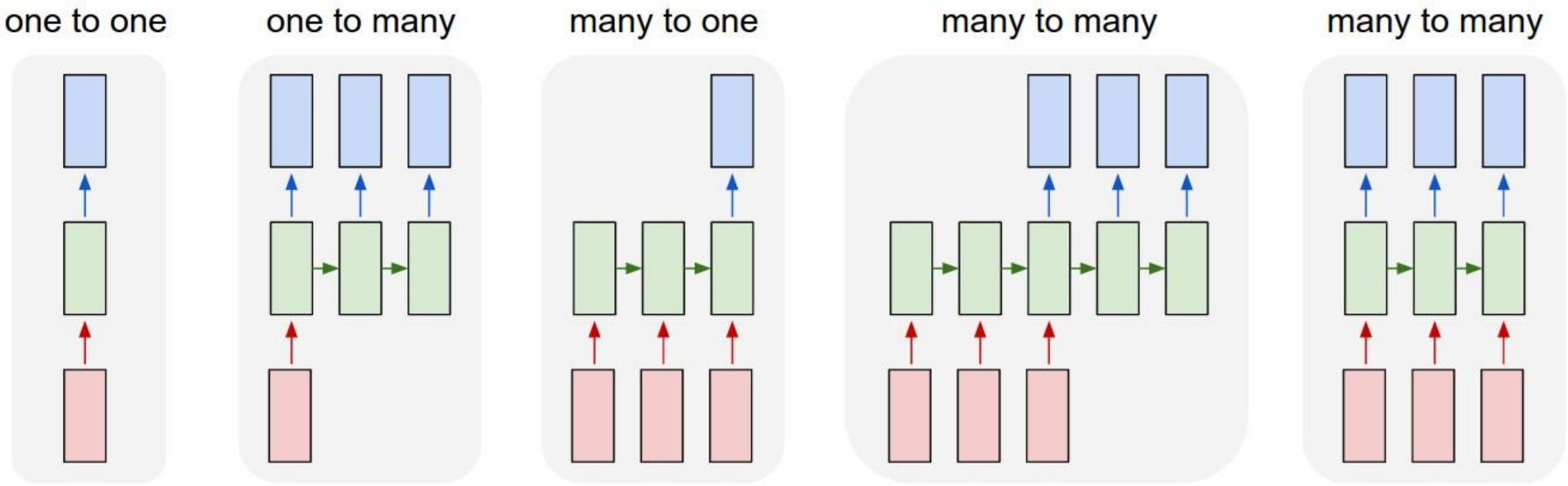
e.g., **Video classification:**
Sequence of images -> label

Recurrent Neural Networks: Process Sequences



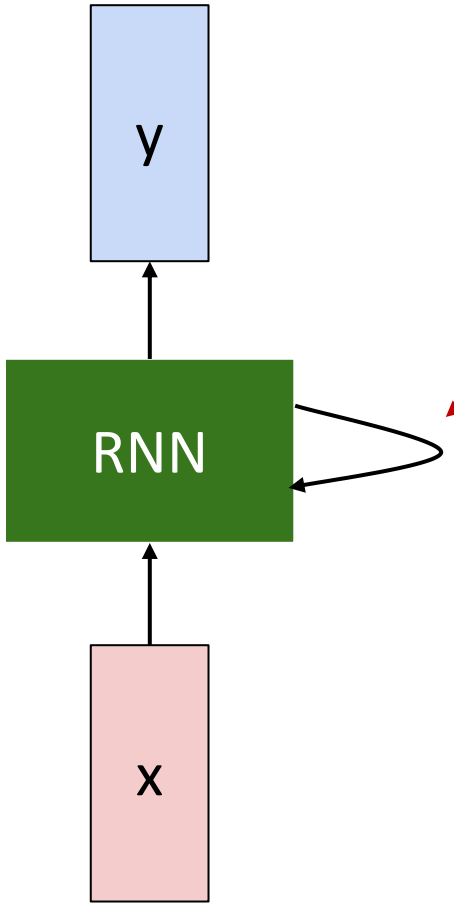
e.g., **Machine Translation:**
Sequence of words -> Sequence of words

Recurrent Neural Networks: Process Sequences



e.g., **Per-frame video classification:**
Sequence of images -> Sequence of labels

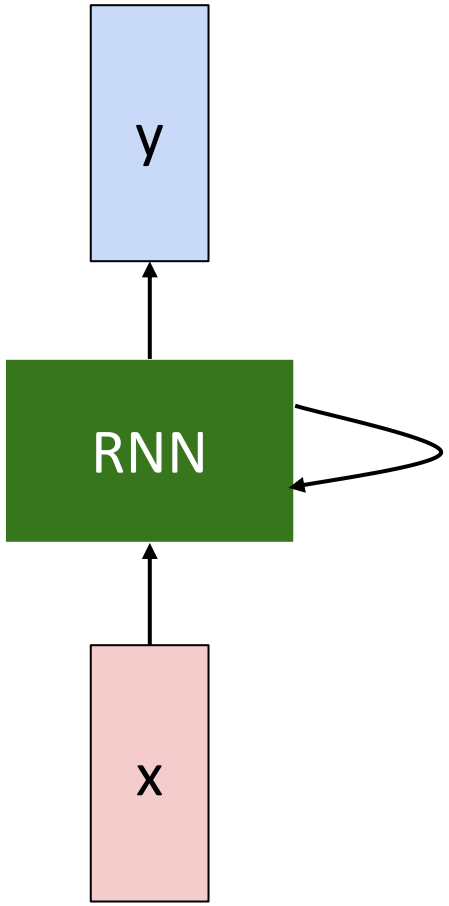
Recurrent Neural Networks



Key idea: RNNs have an "internal state" that is updated as a sequence is processed

Recurrent Neural Networks

Note: the same function and the same set of parameters are used at every time step.



We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:

$$h_t = f_W(h_{t-1}, x_t)$$

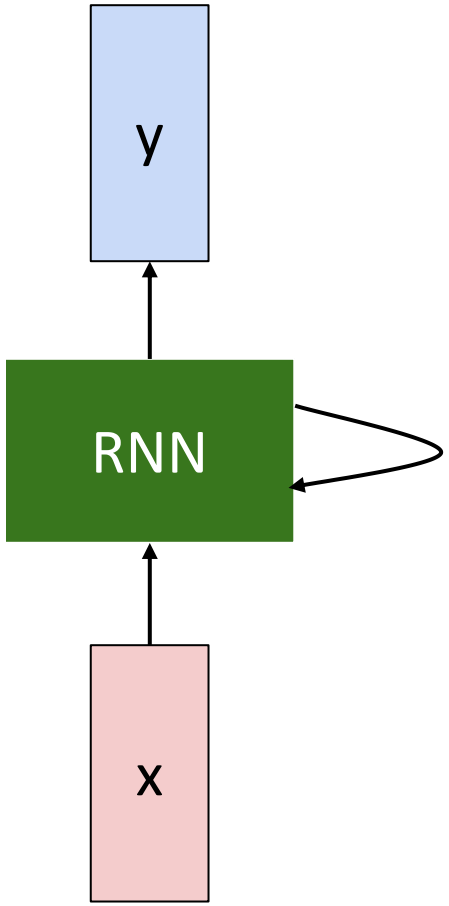
new state

some function with parameters W

old state

input vector at some time step

(Vanilla) Recurrent Neural Networks



The state consists of a single *"hidden"* vector **h**:

$$h_t = f_W(h_{t-1}, x_t)$$

$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t + b_h)$$

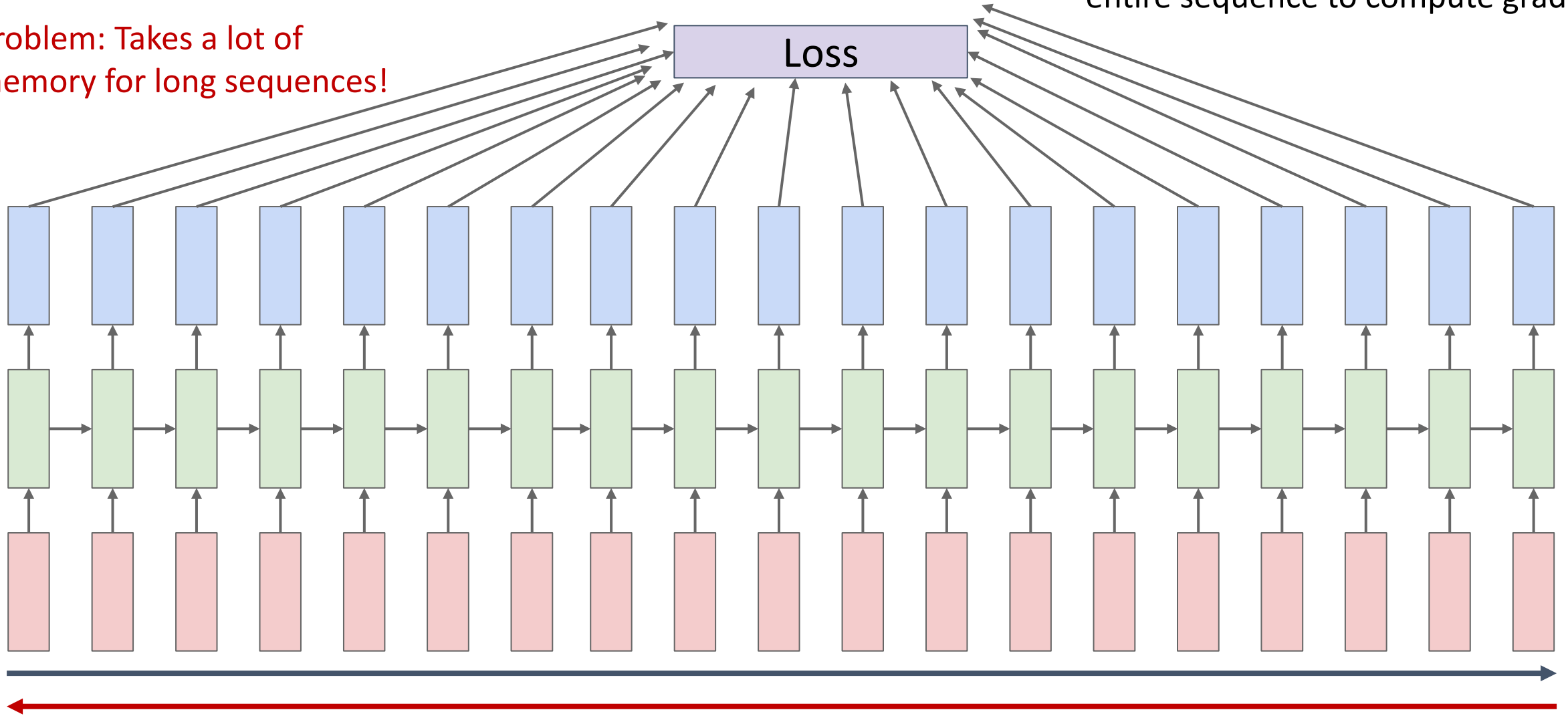
$$y_t = W_{hy}h_t + b_y$$

Sometimes called a "Vanilla RNN" or an "Elman RNN" after Prof. Jeffrey Elman

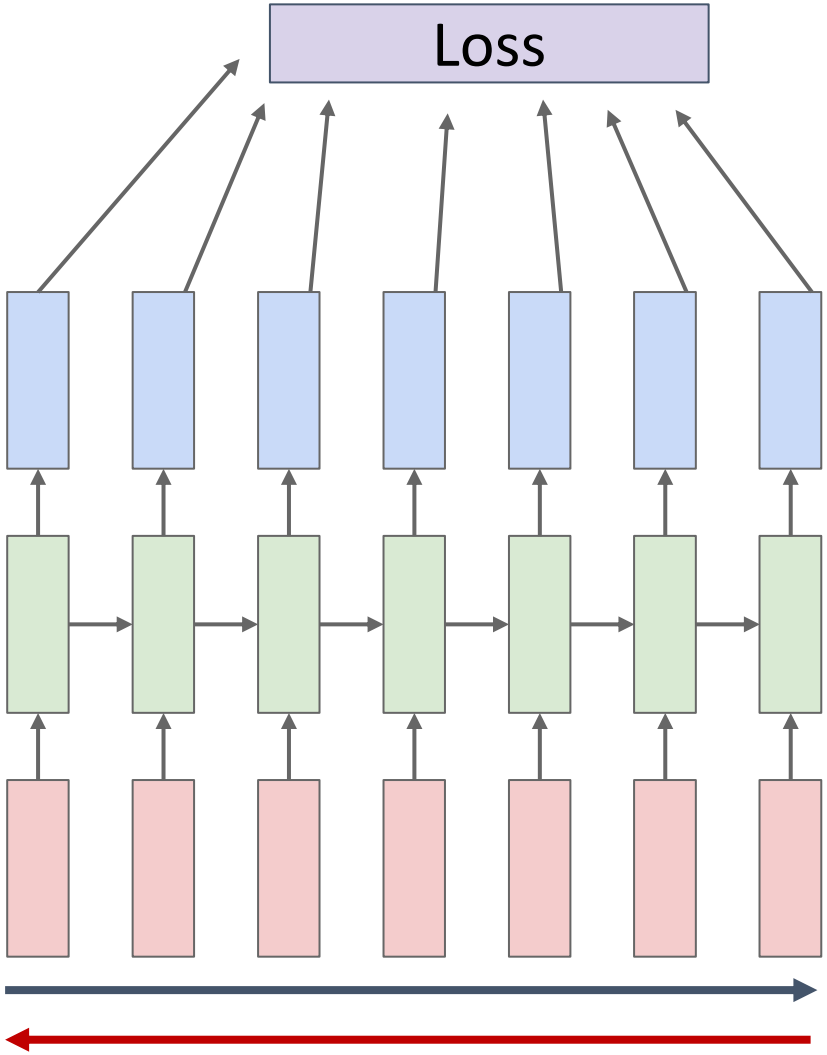
Backpropagation Through Time

Forward through entire sequence to compute loss, then backward through entire sequence to compute gradient

Problem: Takes a lot of memory for long sequences!

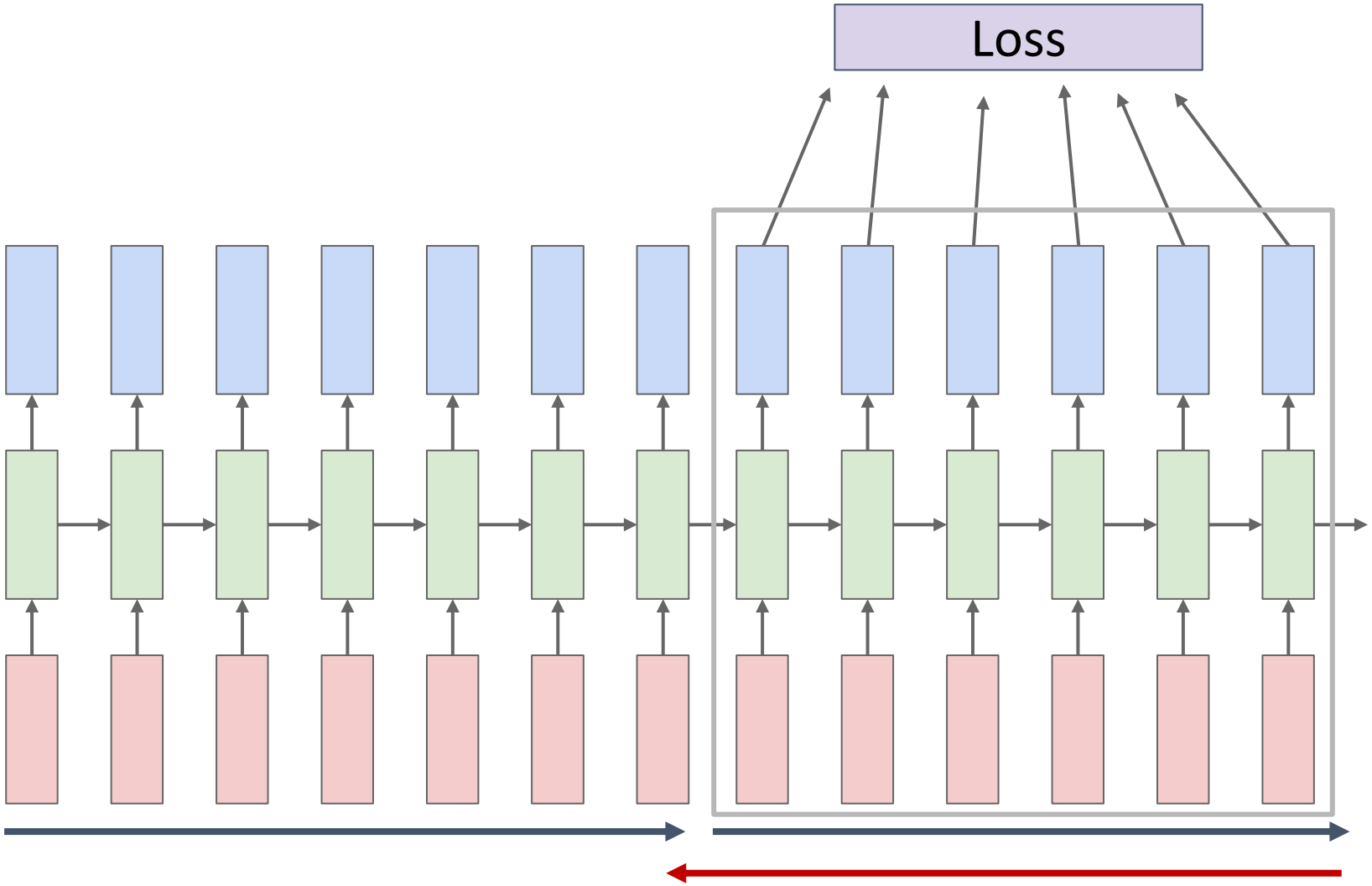


Truncated Backpropagation Through Time



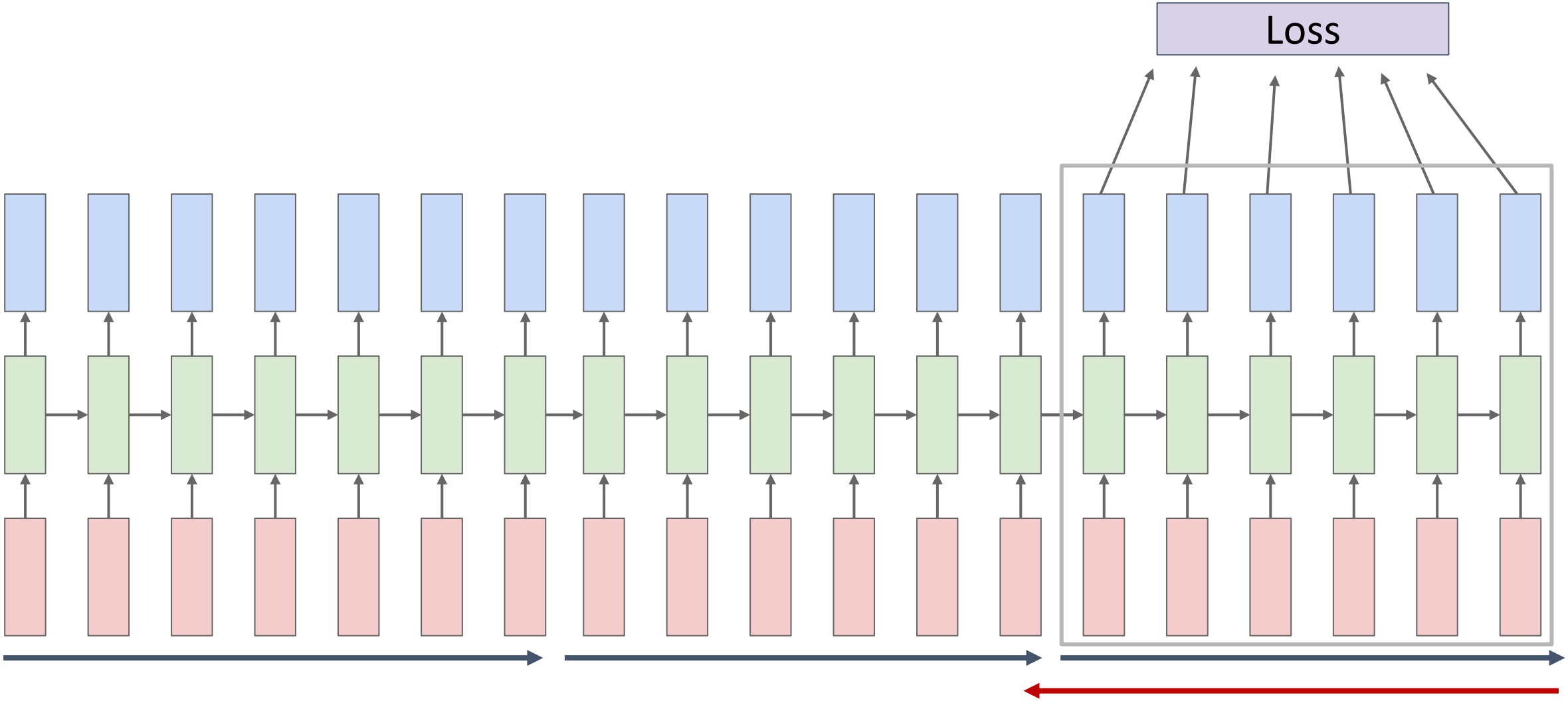
Run forward and backward through chunks of the sequence instead of whole sequence

Truncated Backpropagation Through Time



Carry hidden states forward in time forever, but only backpropagate for some smaller number of steps

Truncated Backpropagation Through Time



Long Short Term Memory (LSTM)

Vanilla RNN

$$h_t = \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h\right)$$

LSTM

$$\begin{pmatrix} i_t \\ f_t \\ o_t \\ g_t \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} \left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h\right)$$

$$c_t = f_t \odot c_{t-1} + i_t \odot g_t$$

$$h_t = o_t \odot \tanh(c_t)$$

Two vectors at each timestep:

Cell state: $c_t \in \mathbb{R}^H$

Hidden state: $h_t \in \mathbb{R}^H$

Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation 1997

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$$c_t = f_t \odot c_{t-1} + i_t \odot g_t$$

$$h_t = o_t \odot \tanh(c_t)$$

Compute four "gates" per timestep:

Input gate: $\mathrm{i}_t \in \mathbb{R}^H$

Forget gate: $\mathrm{f}_t \in \mathbb{R}^H$

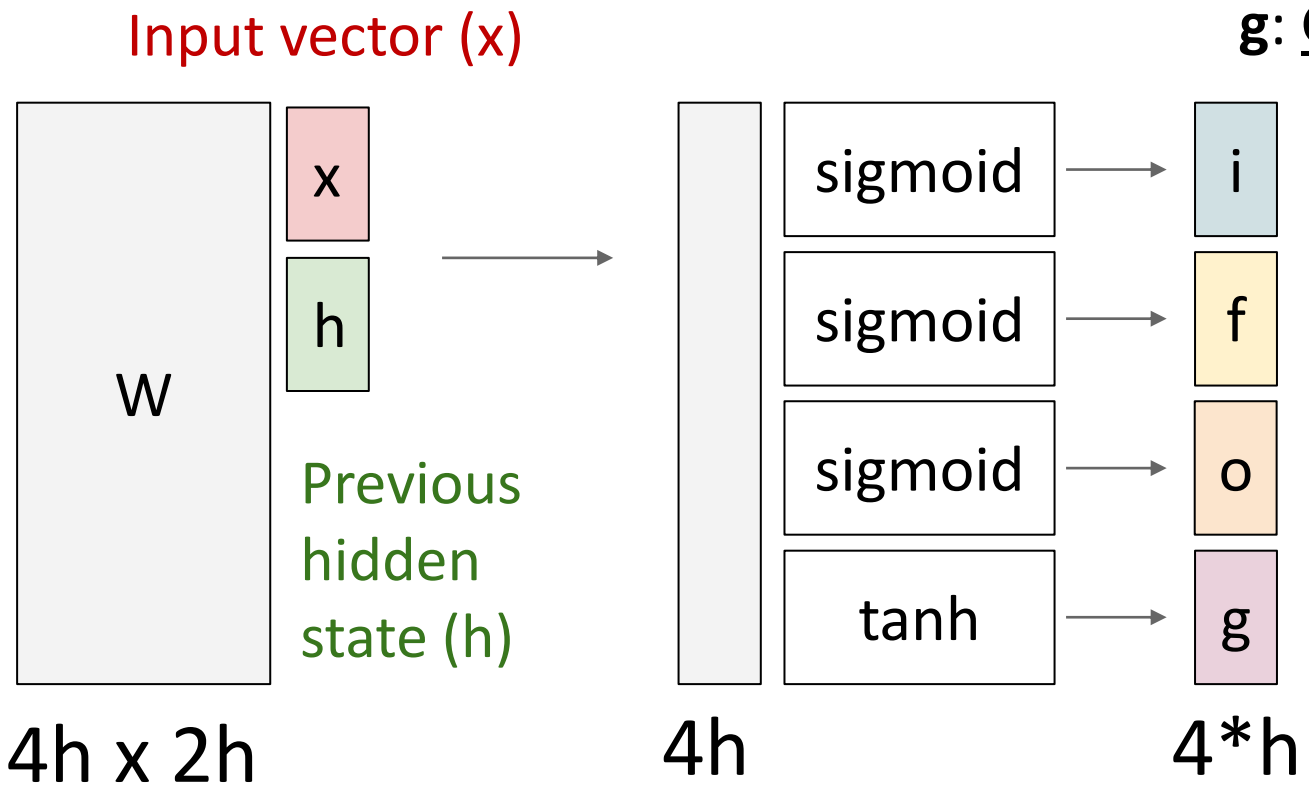
Output gate: $\mathrm{o}_t \in \mathbb{R}^H$

"Gate?" gate: $\mathrm{g}_t \in \mathbb{R}^H$

Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation 1997

Long Short Term Memory (LSTM)

i: Input gate, whether to write to cell
f: Forget gate, Whether to erase cell
o: Output gate, How much to reveal cell
g: Gate gate (?), How much to write to cell



$$\begin{pmatrix} i_t \\ f_t \\ o_t \\ g_t \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} \left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h \right)$$

$$c_t = f_t \odot c_{t-1} + i_t \odot g_t$$

$$h_t = o_t \odot \tanh(c_t)$$

Single-Layer RNNs

$$h_t = \tanh\left(W\begin{pmatrix}h_{t-1}\\ x_t\end{pmatrix} + b_h\right)$$

LSTM:

$$\begin{pmatrix}i_t\\ f_t\\ o_t\\ g_t\end{pmatrix} = \begin{pmatrix}\sigma\\ \sigma\\ \sigma\\ \tanh\end{pmatrix}\left(W\begin{pmatrix}h_{t-1}\\ x_t\end{pmatrix} + b_h\right)$$

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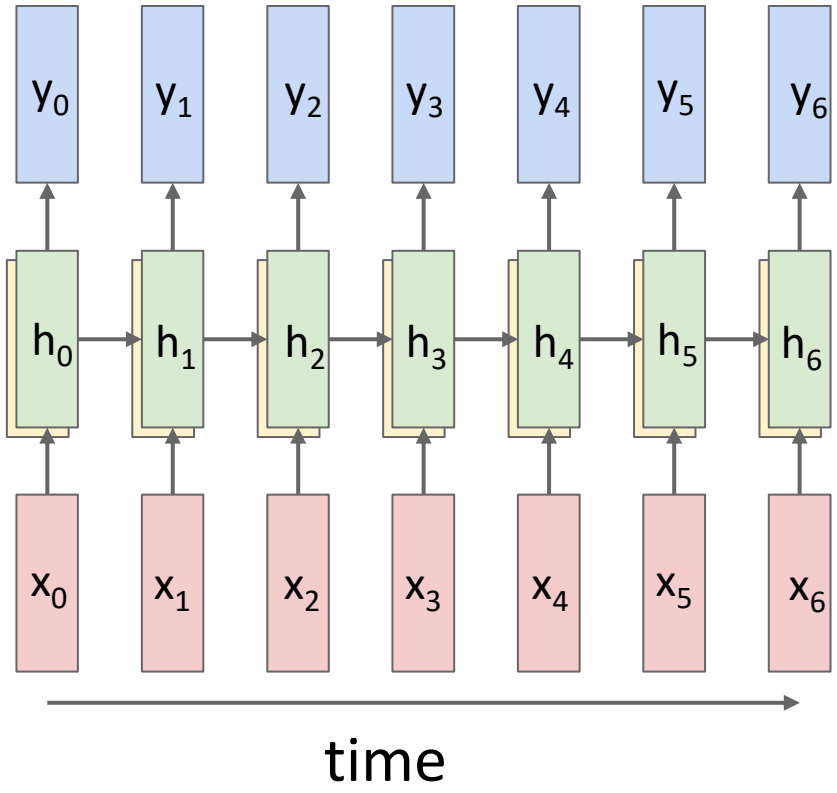


Mutilayer RNNs

$$h_t^\ell = \tanh\left(W\begin{pmatrix}h_{t-1}^\ell \\ h_t^{\ell-1}\end{pmatrix} + b_h^\ell\right)$$

LSTM:

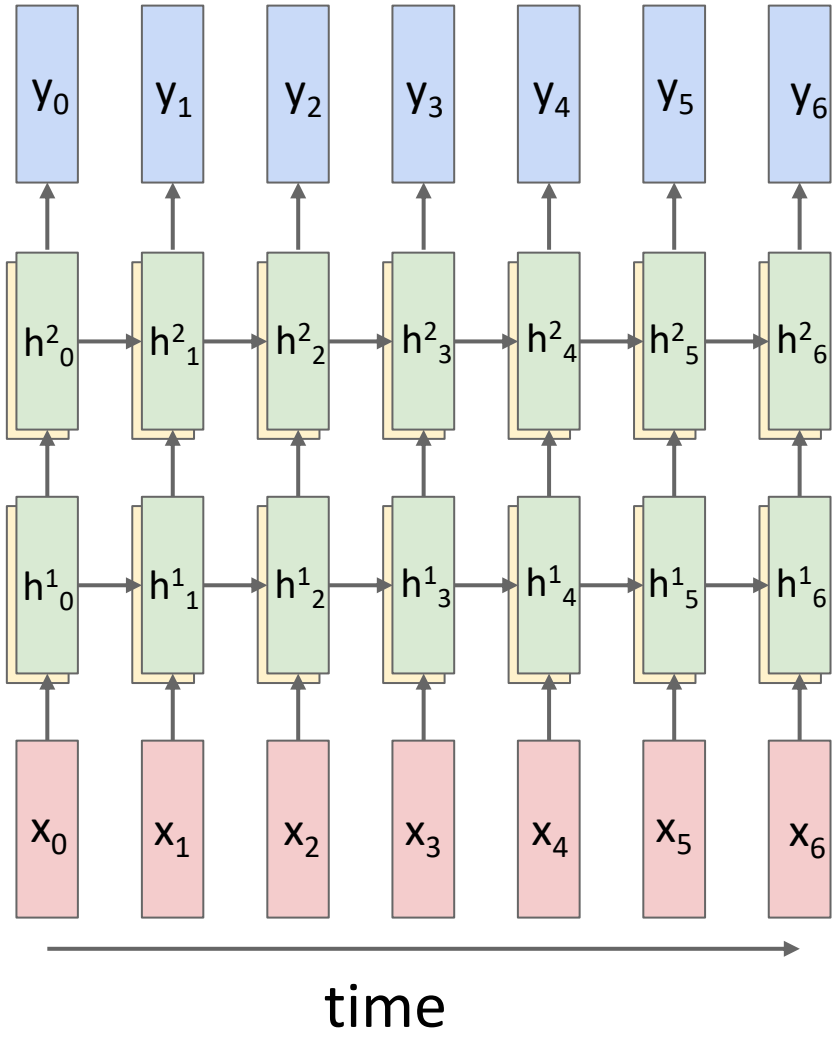
$$\begin{pmatrix}i_t^\ell \\ f_t^\ell \\ o_t^\ell \\ g_t^\ell\end{pmatrix} = \begin{pmatrix}\sigma \\ \sigma \\ \sigma \\ \tanh\end{pmatrix}\left(W\begin{pmatrix}h_{t-1}^\ell \\ h_t^{\ell-1}\end{pmatrix} + b_h^\ell\right)$$

$$c_t^\ell = f_t^\ell \odot c_{t-1}^\ell + i_t^\ell \odot g_t^\ell$$

$$h_t^\ell = o_t^\ell \odot \tanh(c_t^\ell)$$

depth

Two-layer RNN: Pass hidden states from one RNN as inputs to another RNN



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LSTM:

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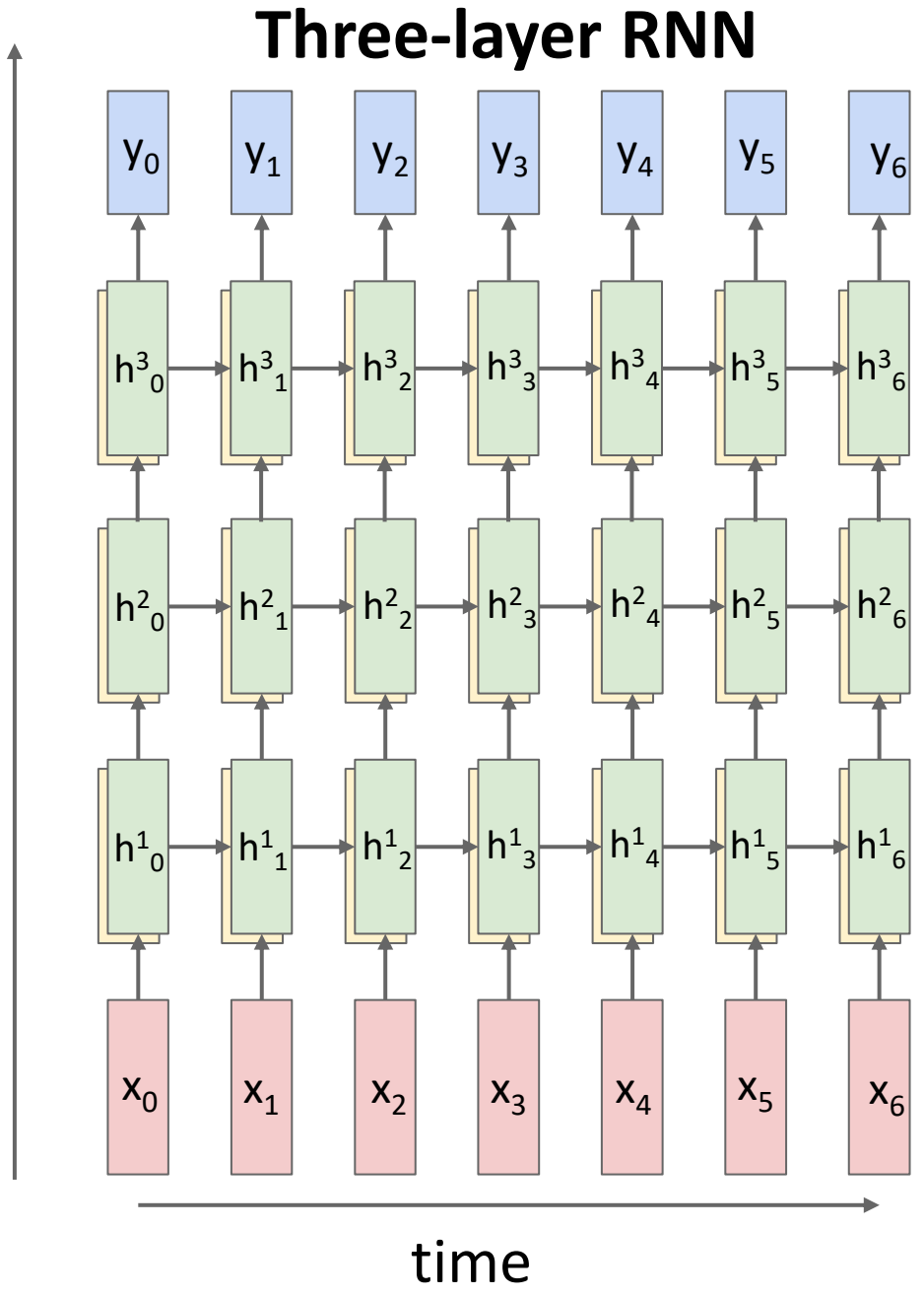
$$c_t^\ell = f_t^\ell \odot c_{t-1}^\ell + i_t^\ell \odot g_t^\ell$$

$$h_t^\ell = o_t^\ell \odot \tanh(c_t^\ell)$$



Other RNN Variants

Gated Recurrent Unit (GRU)

Cho et al. “Learning phrase representations using RNN encoder-decoder for statistical machine translation”, 2014

$$r_t = \sigma(W_{xr}x_t + W_{hr}h_{t-1} + b_r)$$
$$z_t = \sigma(W_{xz}x_t + W_{hz}h_{t-1} + b_z)$$
$$\tilde{h}_t = \tanh(W_{xh}x_t + W_{hh}(r_T \odot h_{t-1}) + b_h)$$
$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t$$

Other RNN Variants

10,000 architectures with evolutionary search:
Jozefowicz et al, "An empirical exploration of recurrent network architectures", ICML 2015

Gated Recurrent Unit (GRU)
Cho et al. "Learning phrase representations using RNN encoder-decoder for statistical machine translation", 2014

$$r_t = \sigma(W_{xr}x_t + W_{hr}h_{t-1} + b_r)$$
$$z_t = \sigma(W_{xz}x_t + W_{hz}h_{t-1} + b_z)$$
$$\tilde{h}_t = \tanh(W_{xh}x_t + W_{hh}(r_T \odot h_{t-1}) + b_h)$$
$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t$$

MUT1:

$$\begin{aligned} z &= \text{sigm}(W_{\text{xz}}x_t + b_{\text{z}}) \\ r &= \text{sigm}(W_{\text{xr}}x_t + W_{\text{hr}}h_t + b_{\text{r}}) \\ h_{t+1} &= \tanh(W_{\text{hh}}(r \odot h_t) + \tanh(x_t) + b_{\text{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT2:

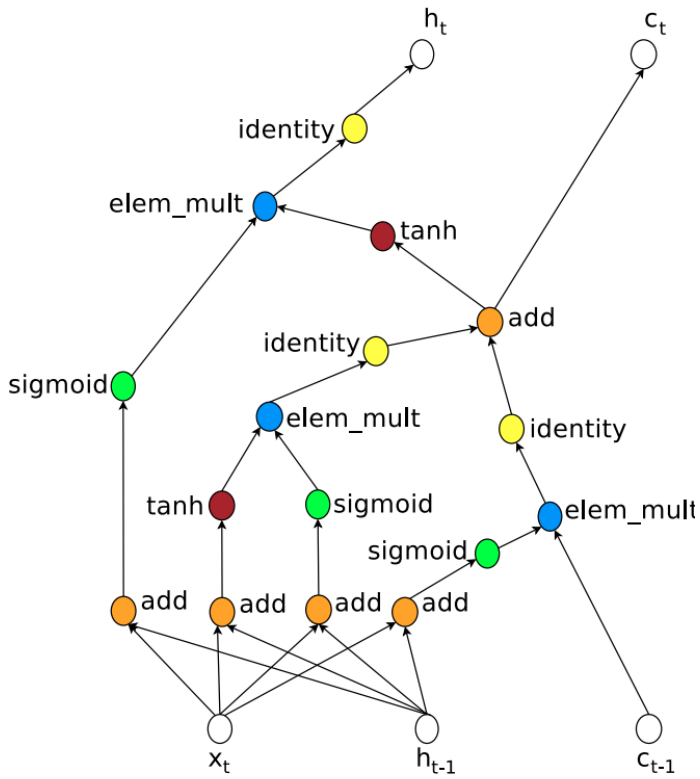
$$\begin{aligned} z &= \text{sigm}(W_{\text{xz}}x_t + W_{\text{hz}}h_t + b_{\text{z}}) \\ r &= \text{sigm}(x_t + W_{\text{hr}}h_t + b_{\text{r}}) \\ h_{t+1} &= \tanh(W_{\text{hh}}(r \odot h_t) + W_{xh}x_t + b_{\text{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT3:

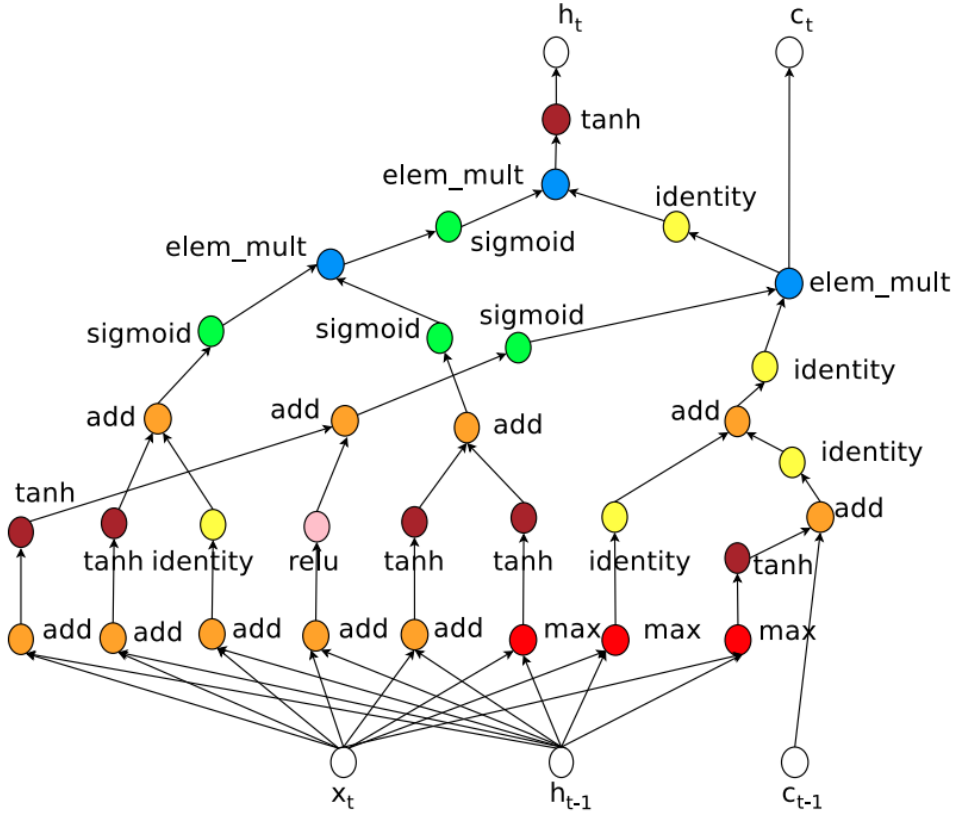
$$\begin{aligned} z &= \text{sigm}(W_{\text{xz}}x_t + W_{\text{hz}}\tanh(h_t) + b_{\text{z}}) \\ r &= \text{sigm}(W_{\text{xr}}x_t + W_{\text{hr}}h_t + b_{\text{r}}) \\ h_{t+1} &= \tanh(W_{\text{hh}}(r \odot h_t) + W_{xh}x_t + b_{\text{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

RNN Architectures: Neural Architecture Search

LSTM



Learned Architecture



Zoph and Le, "Neural Architecture Search with Reinforcement Learning", ICLR 2017

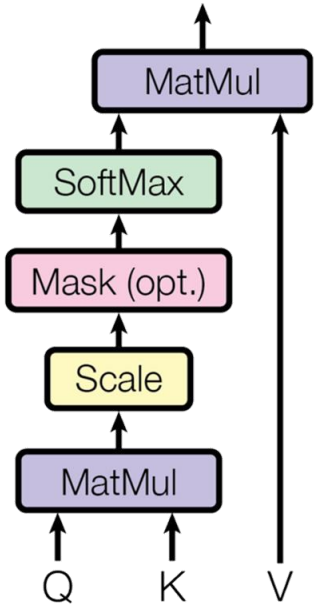
Outline

- Recurrent Neural Networks
- Attention and Transformers
- Vision Transformers

Attention

- Mapping a query and a set of key-value pairs to an output, where the query, keys, values, and output are all vectors

- Scaled Dot-Product Attention:



$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{D_Q}}\right)V$$

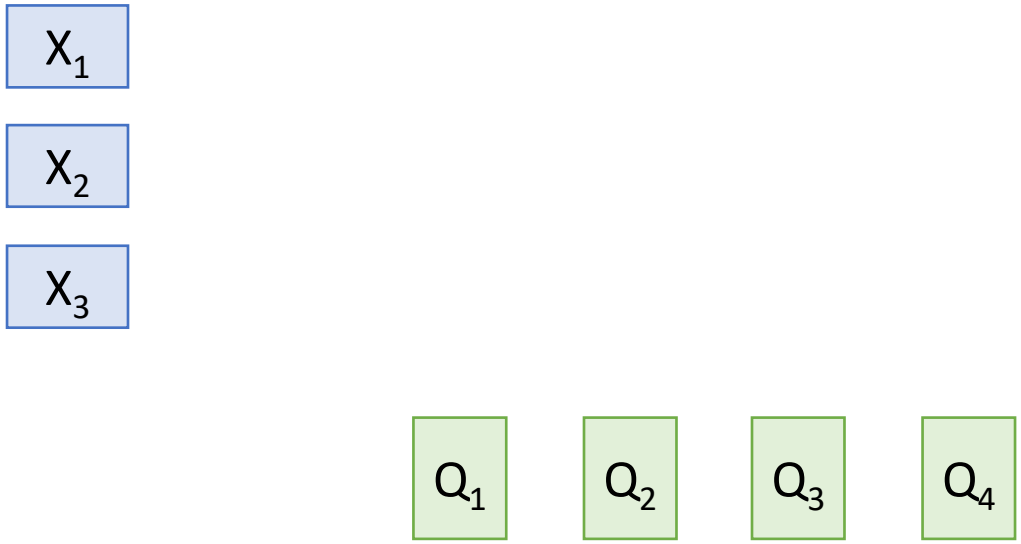
Caution: In the following slides, weight matrix multiplications mostly come with bias addition but omitted

Vaswani et al, "Attention is all you need", NeurIPS 2017

Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

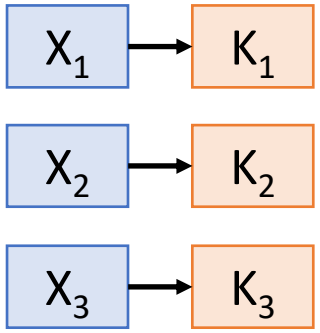
Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

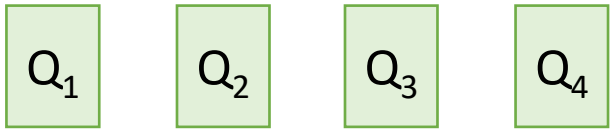


Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$





Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
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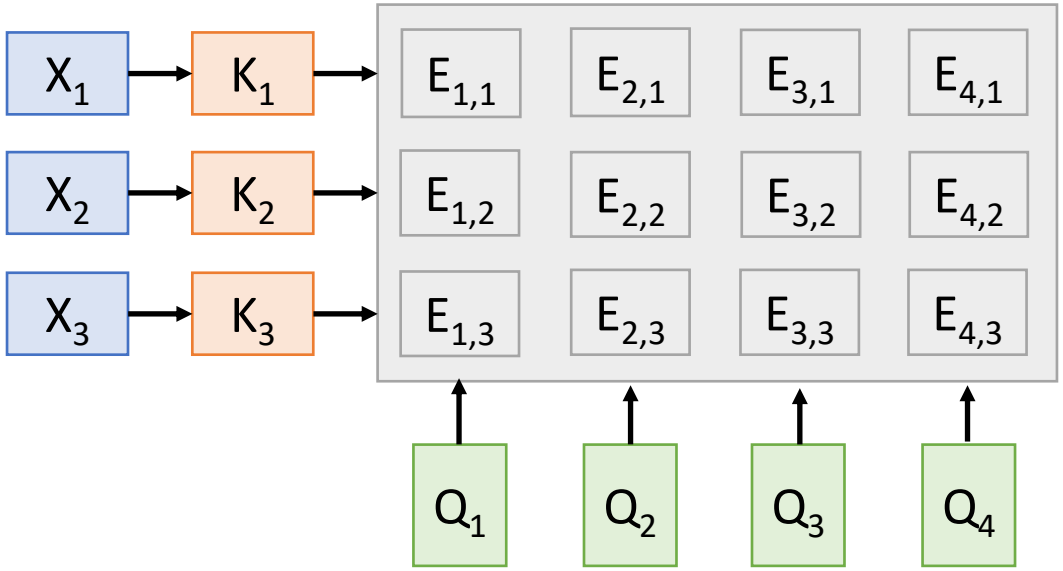
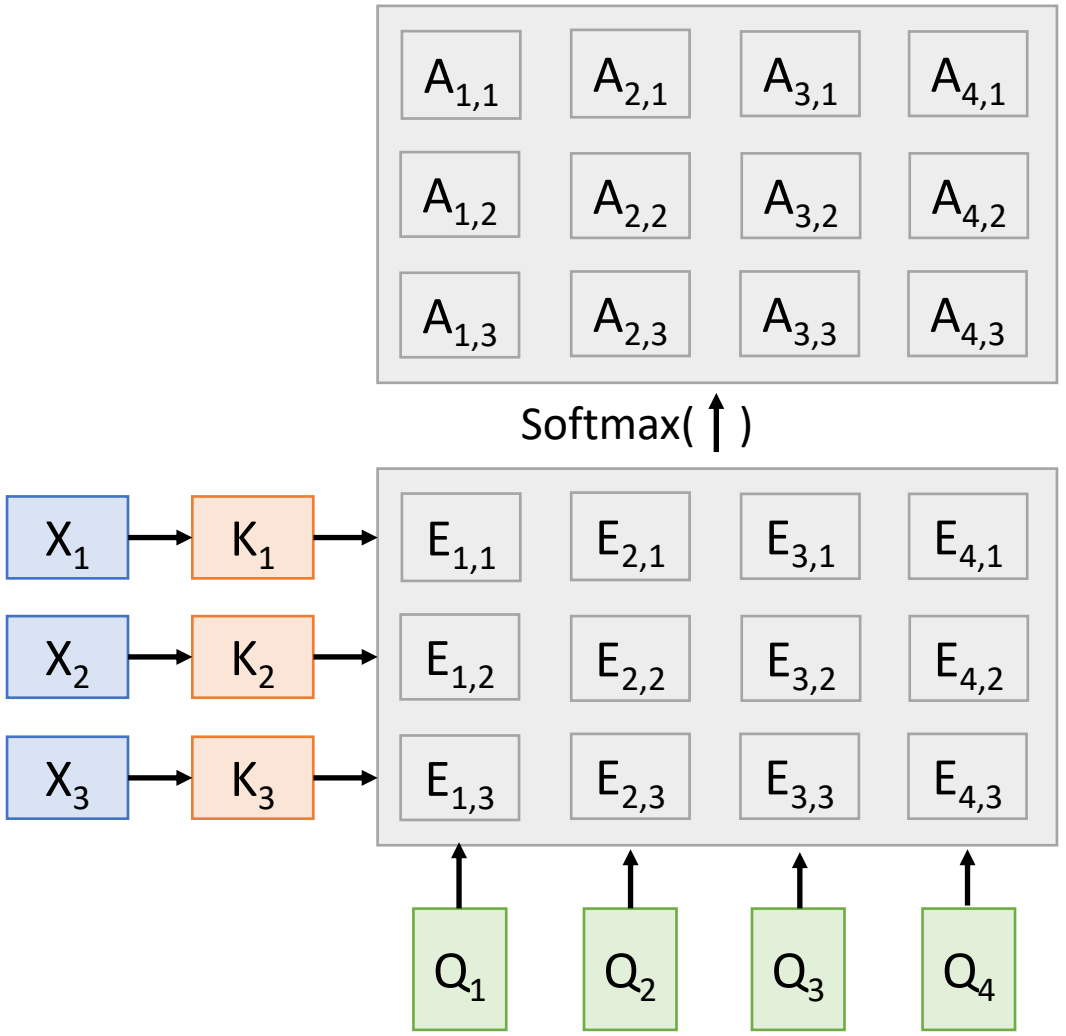


Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



Attention Layer

Inputs:
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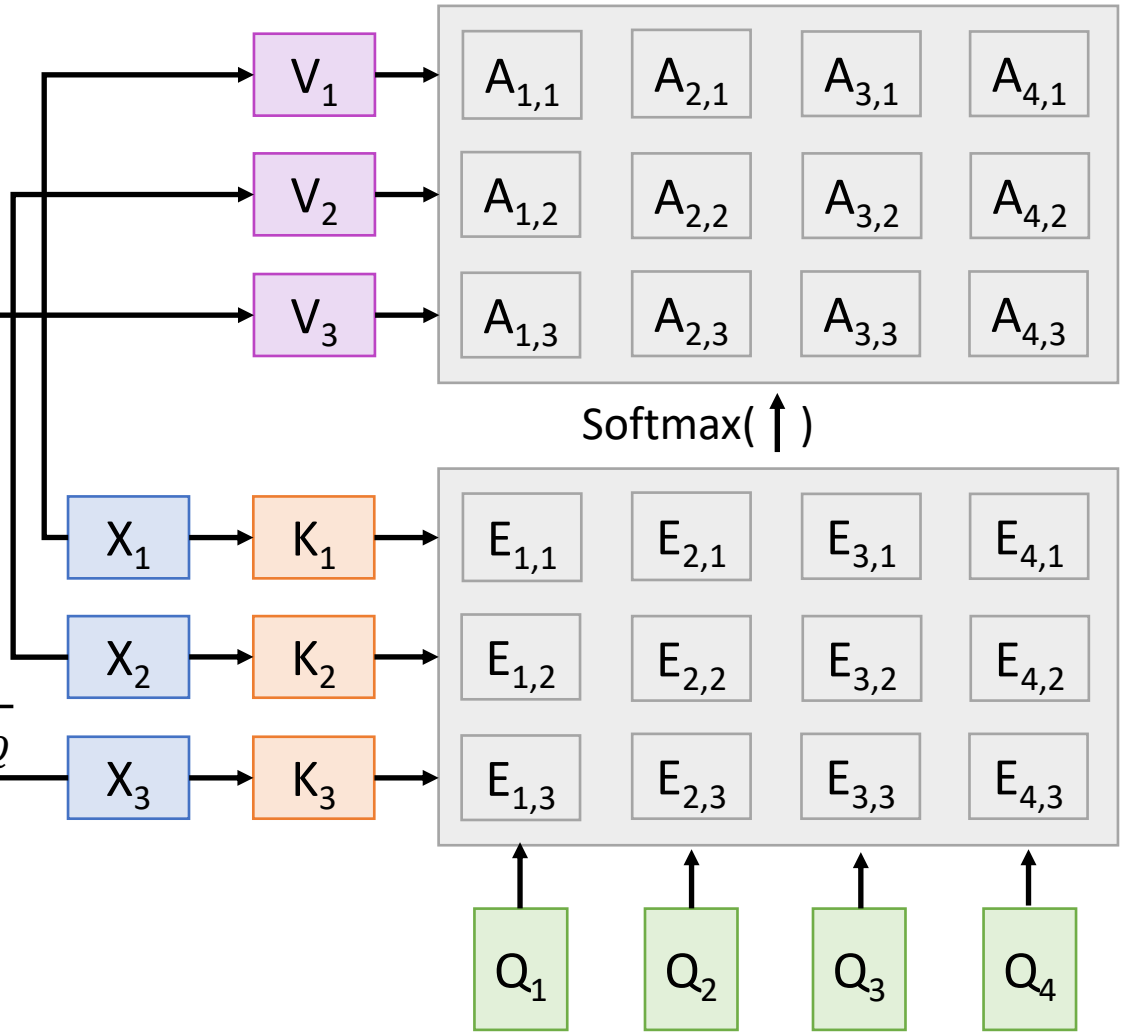
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

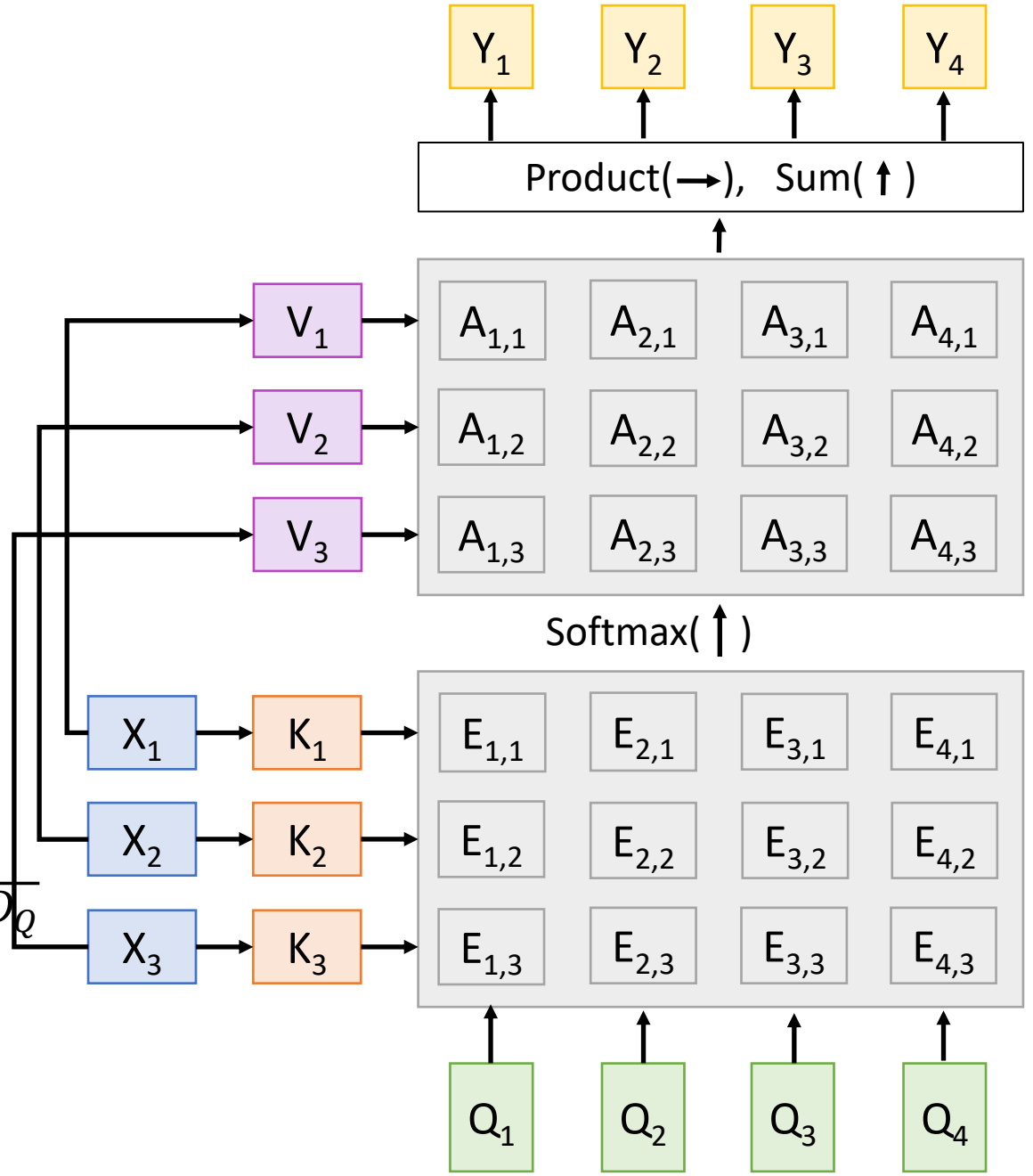
Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$



Attention Layer

Inputs:
Query vectors: Q (Shape: N_Q x D_Q)
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)

Computation:
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: Y = AV (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} V_j$

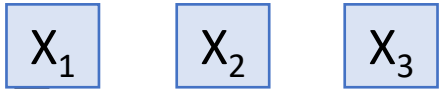


Self-Attention Layer

One **query** per **input vector**

Inputs:
Query vectors: **Q** (Shape: N_Q x D_Q)
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: $\mathbf{W_K}$ (Shape: D_X x D_Q)
Value matrix: $\mathbf{W_V}$ (Shape: D_X x D_V)

Computation:
Key vectors: $\mathbf{K} = \mathbf{X}\mathbf{W_K}$ (Shape: N_X x D_Q)
Value Vectors: $\mathbf{V} = \mathbf{X}\mathbf{W_V}$ (Shape: N_X x D_V)
Similarities: $E = \mathbf{Q}\mathbf{K}^T / \sqrt{D_Q}$ (Shape: N_Q x N_X) $E_{i,j} = (\mathbf{Q}_i \cdot \mathbf{K}_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_Q x N_X)
Output vectors: $Y = A\mathbf{V}$ (Shape: N_Q x D_V) $Y_i = \sum_j A_{i,j} \mathbf{V}_j$

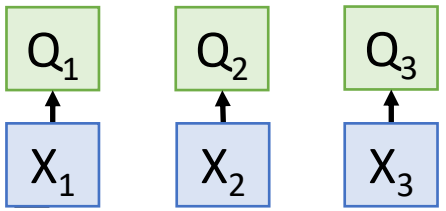


Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

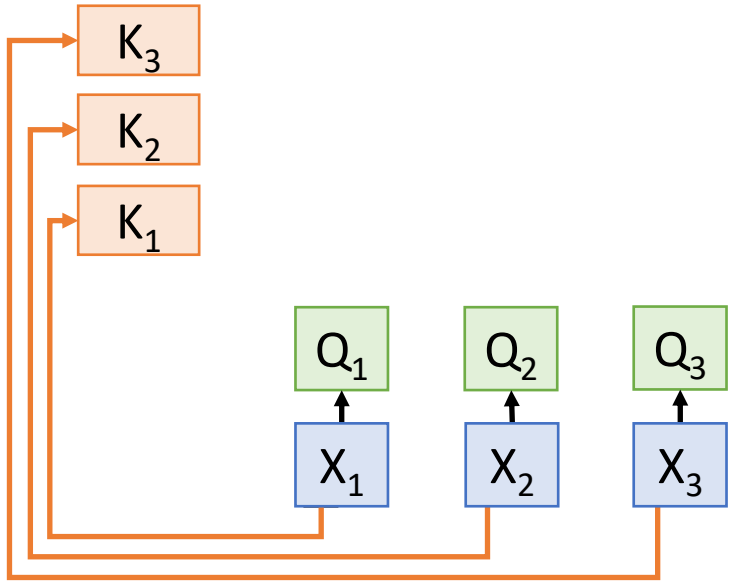


Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

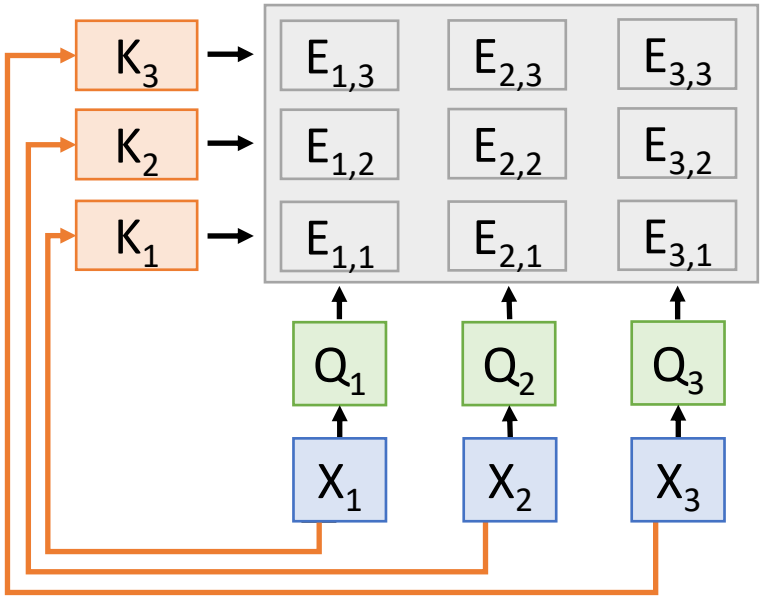


Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

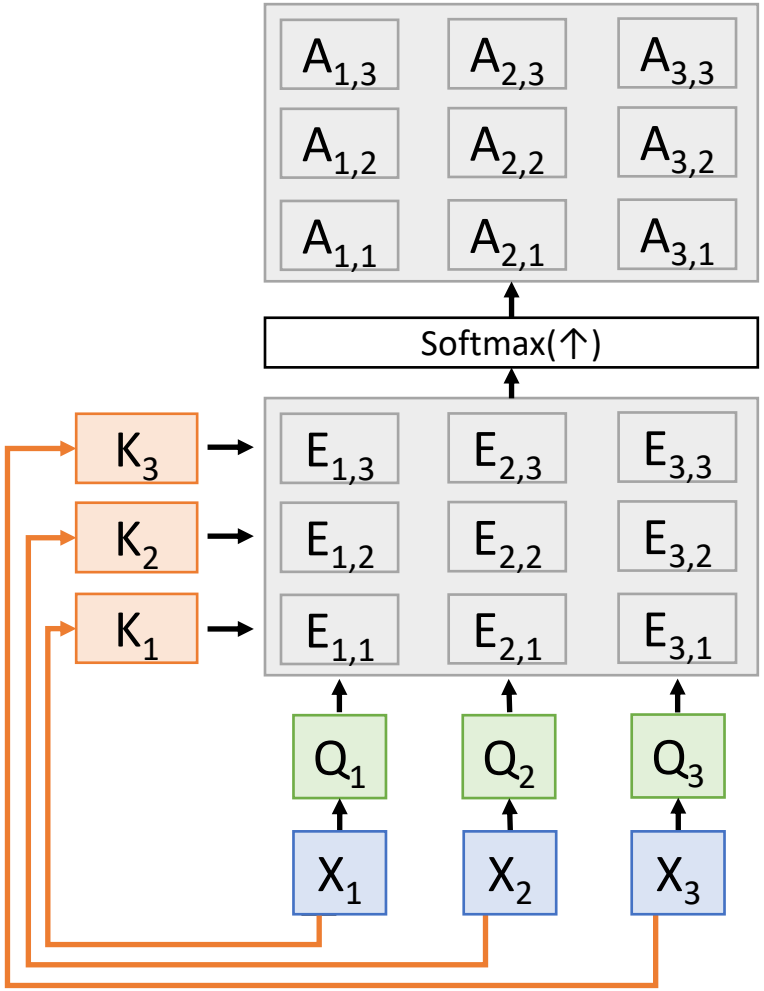


Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

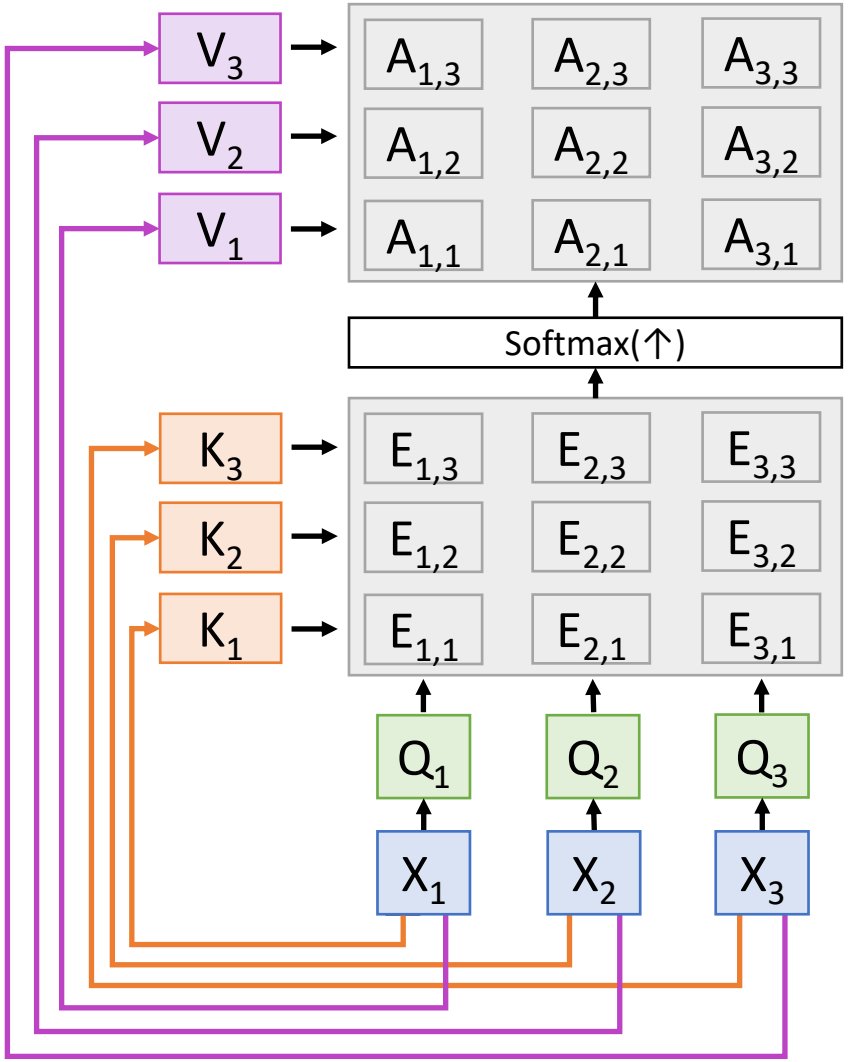


Self-Attention Layer

One **query** per **input vector**

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Self-Attention Layer

One **query** per **input vector**

Inputs:

Input vectors: **X** (Shape: N_X x D_X)

Key matrix: W_K (Shape: D_X x D_Q)

Value matrix: W_V (Shape: D_X x D_V)

Query matrix: W_Q (Shape: D_X x D_Q)

Computation:

Query vectors: $Q = XW_Q$

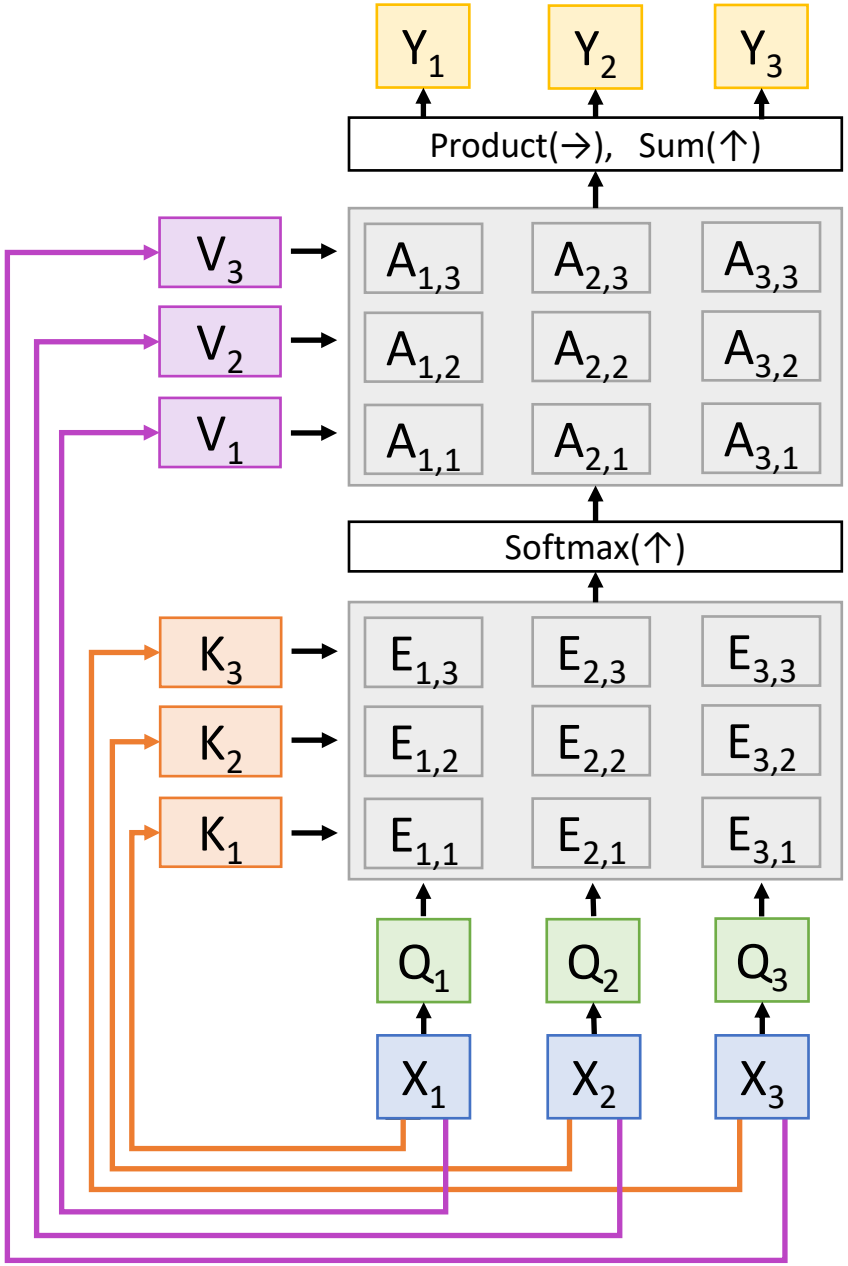
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)

Value Vectors: $V = XW_V$ (Shape: N_X x D_V)

Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$

Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)

Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

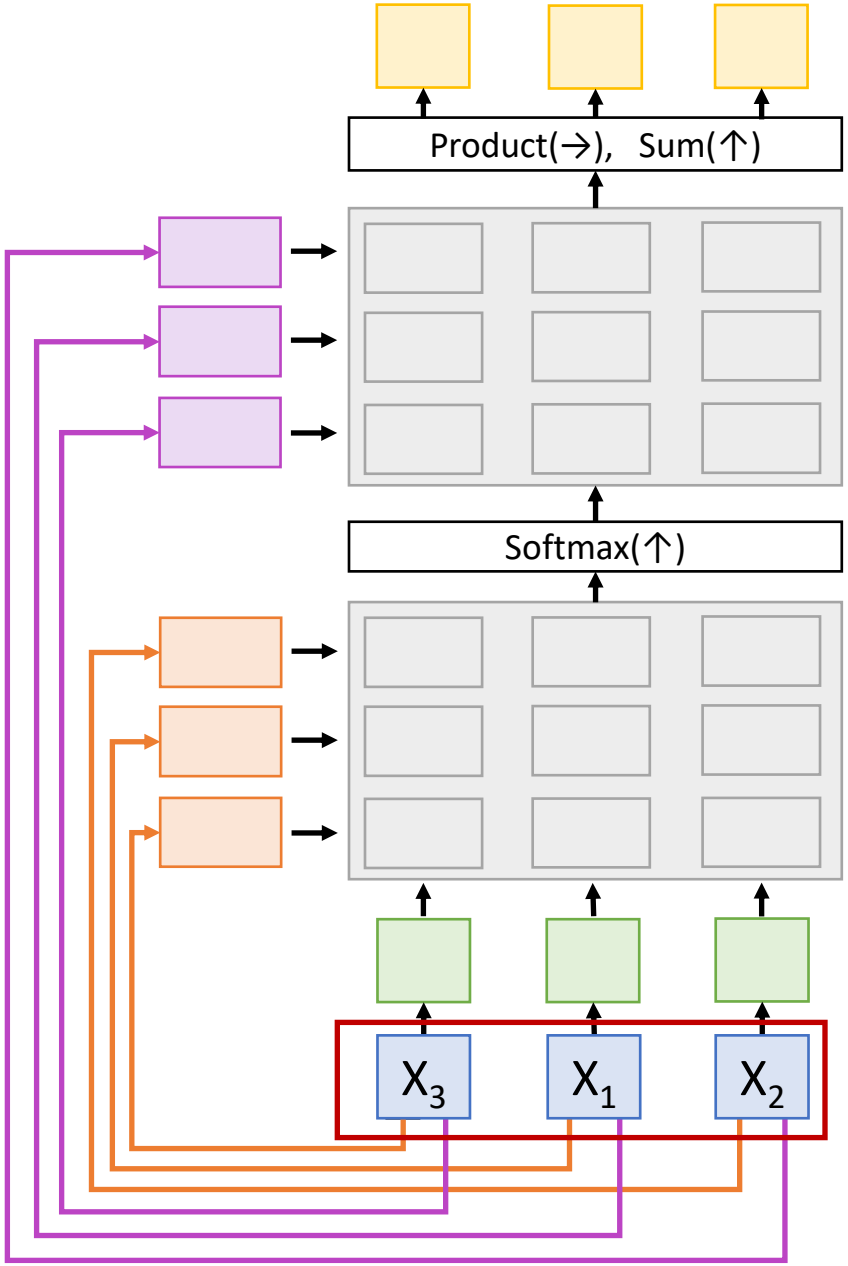


Self-Attention Layer

Consider **permuting** the input vectors:

Inputs:
Input vectors: X (Shape: $N_X \times D_X$)
Key matrix: W_K (Shape: $D_X \times D_Q$)
Value matrix: W_V (Shape: $D_X \times D_V$)
Query matrix: W_Q (Shape: $D_X \times D_Q$)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)
Value Vectors: $V = XW_V$ (Shape: $N_X \times D_V$)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: $N_X \times N_X$) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)
Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



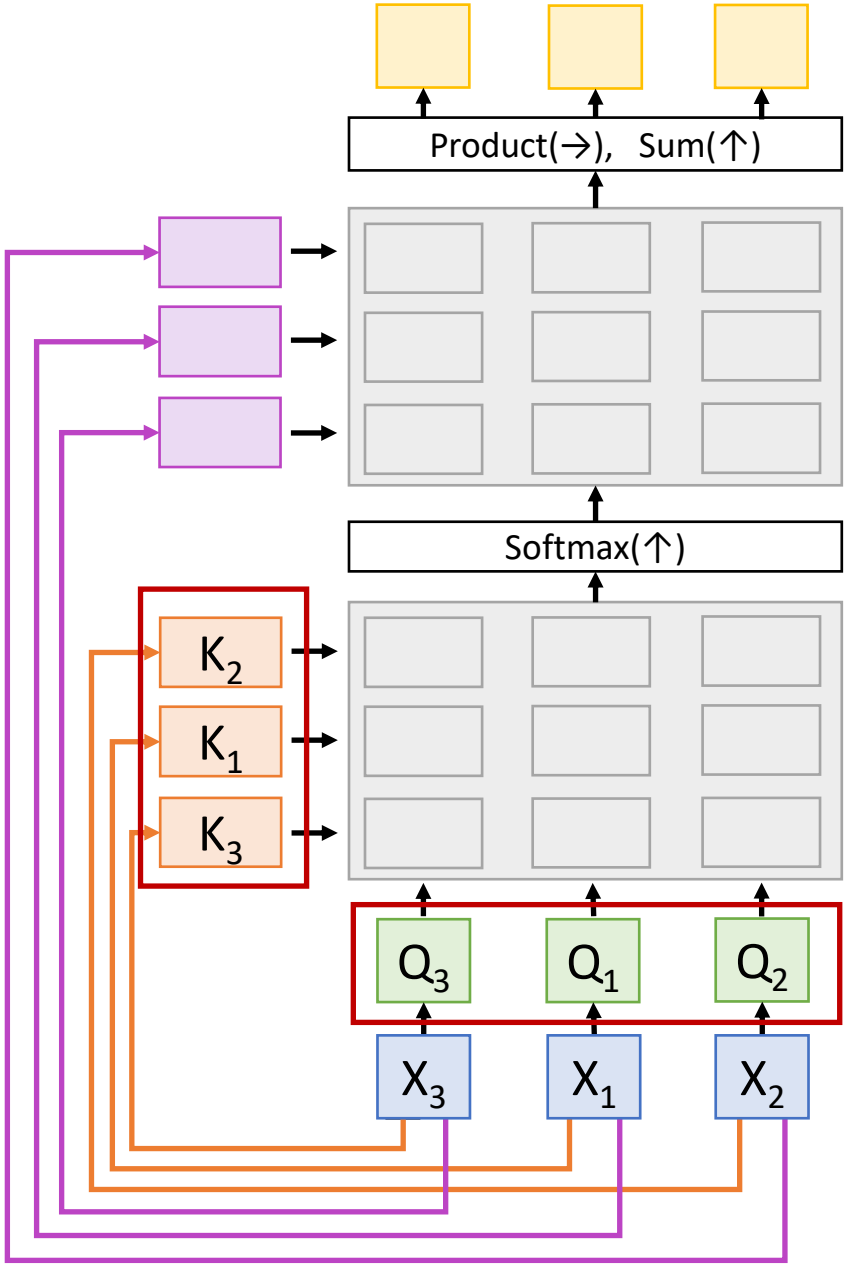
Self-Attention Layer

Consider **permuting** the input vectors:

Queries and Keys will be the same, but permuted

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



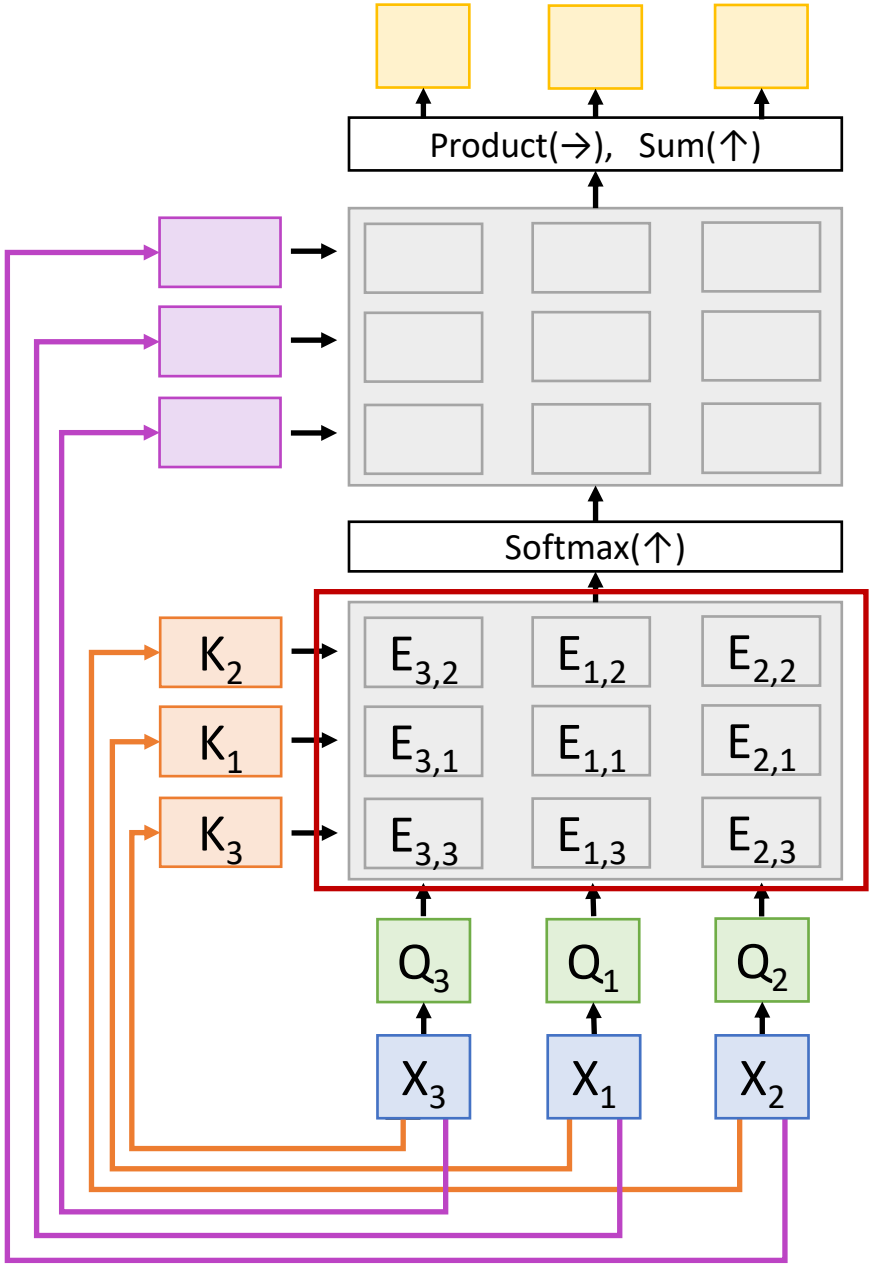
Self-Attention Layer

Consider **permuting** the input vectors:

Similarities will be the same, but permuted

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



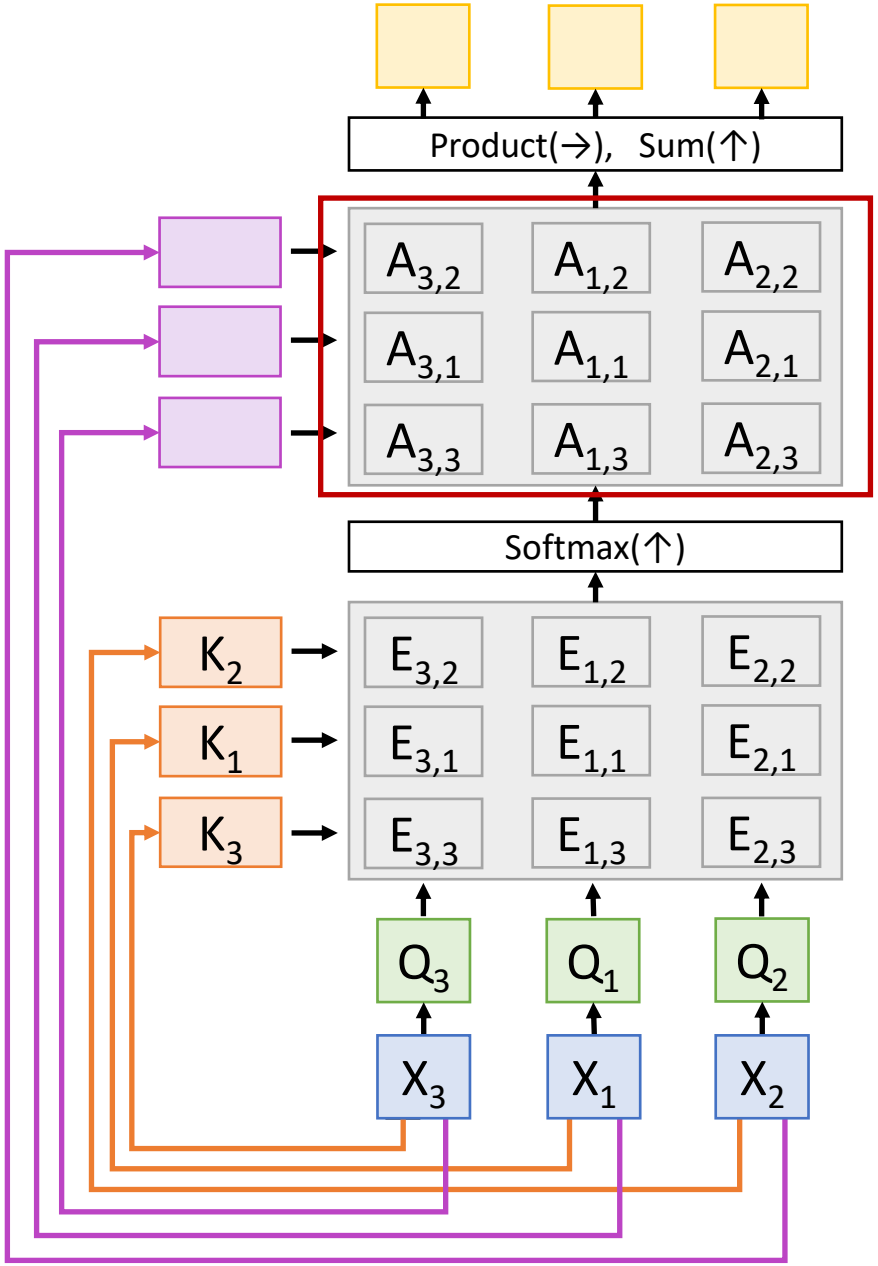
Self-Attention Layer

Consider **permuting** the input vectors:

Attention weights will be the same, but permuted

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



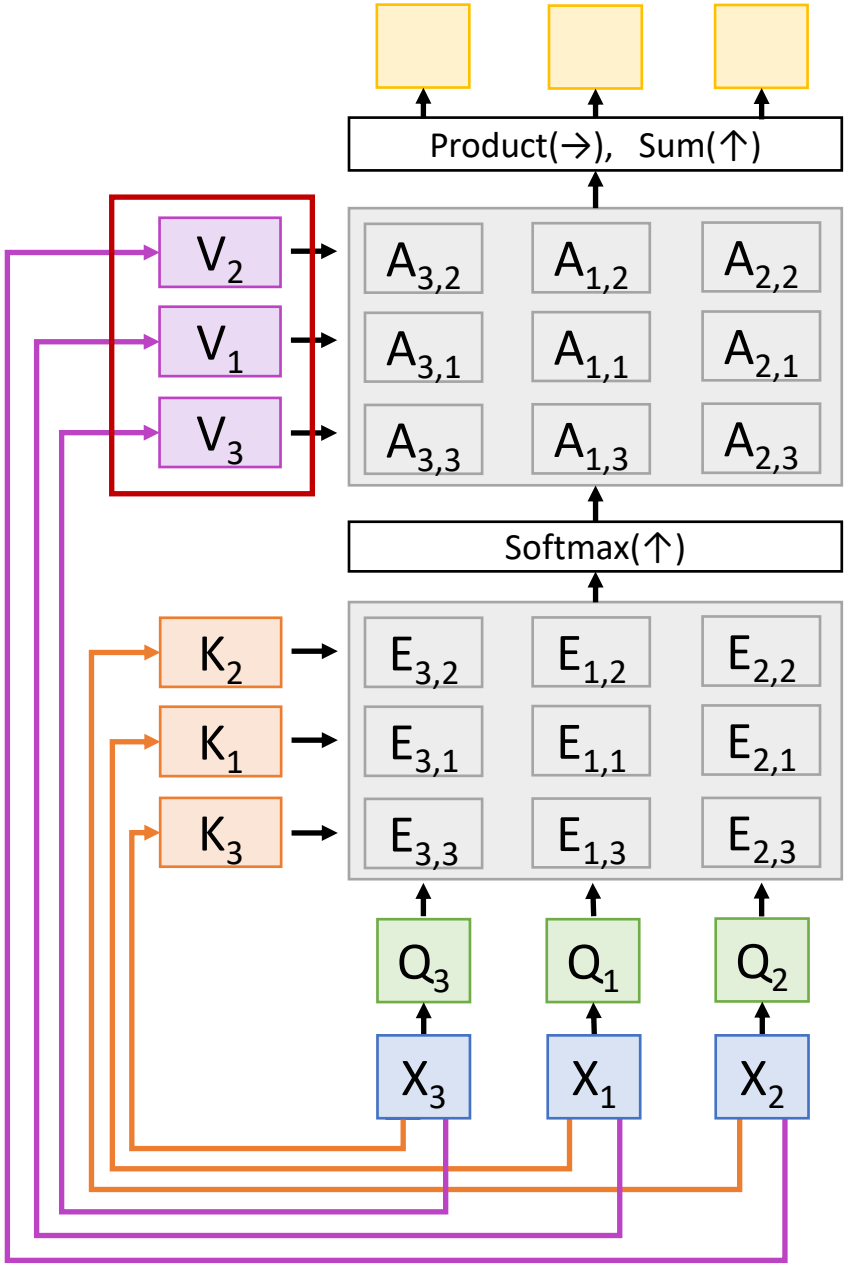
Self-Attention Layer

Consider **permuting** the input vectors:

Values will be the same, but permuted

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Self-Attention Layer

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

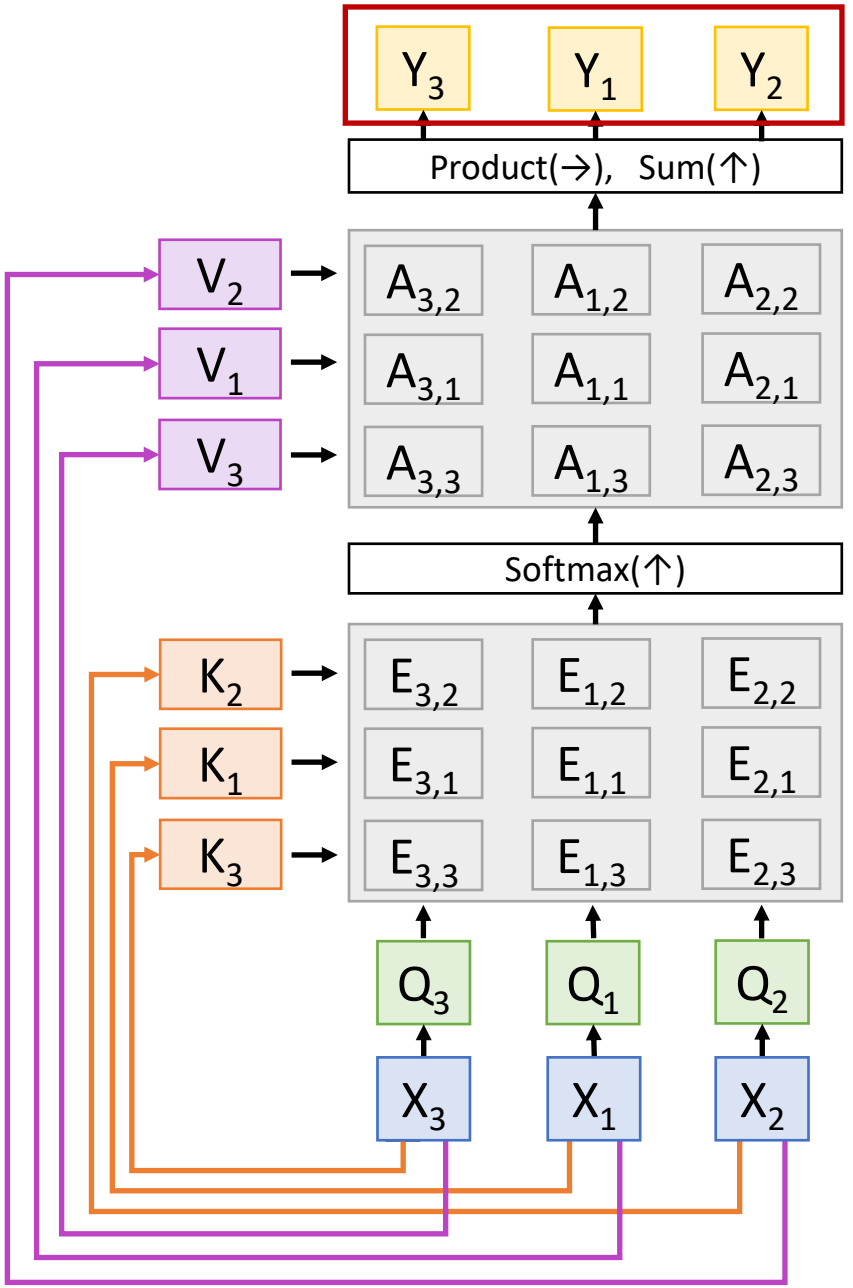
Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

Consider **permuting** the input vectors:

Outputs will be the same, but permuted

Self-attention layer is **Permutation Equivariant**
f(s(x)) = s(f(x))

Self-Attention layer works on **sets** of vectors

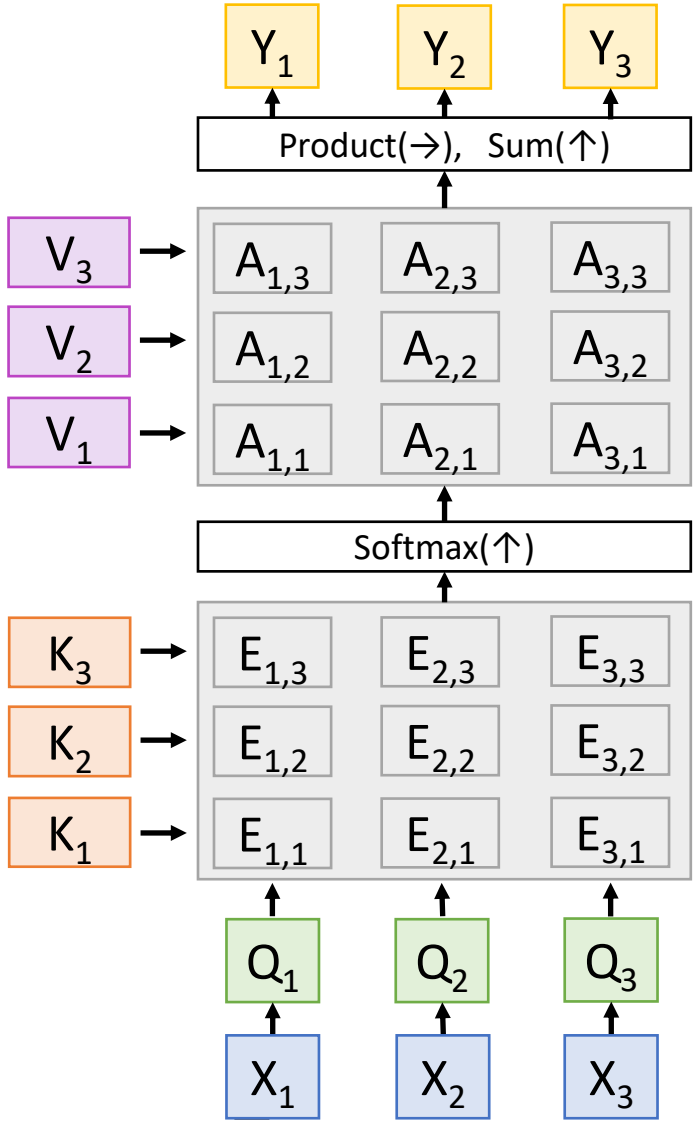


Self-Attention Layer

Self attention doesn't "know" the order of the vectors it is processing!

Inputs:
Input vectors: **X** (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Self-Attention Layer

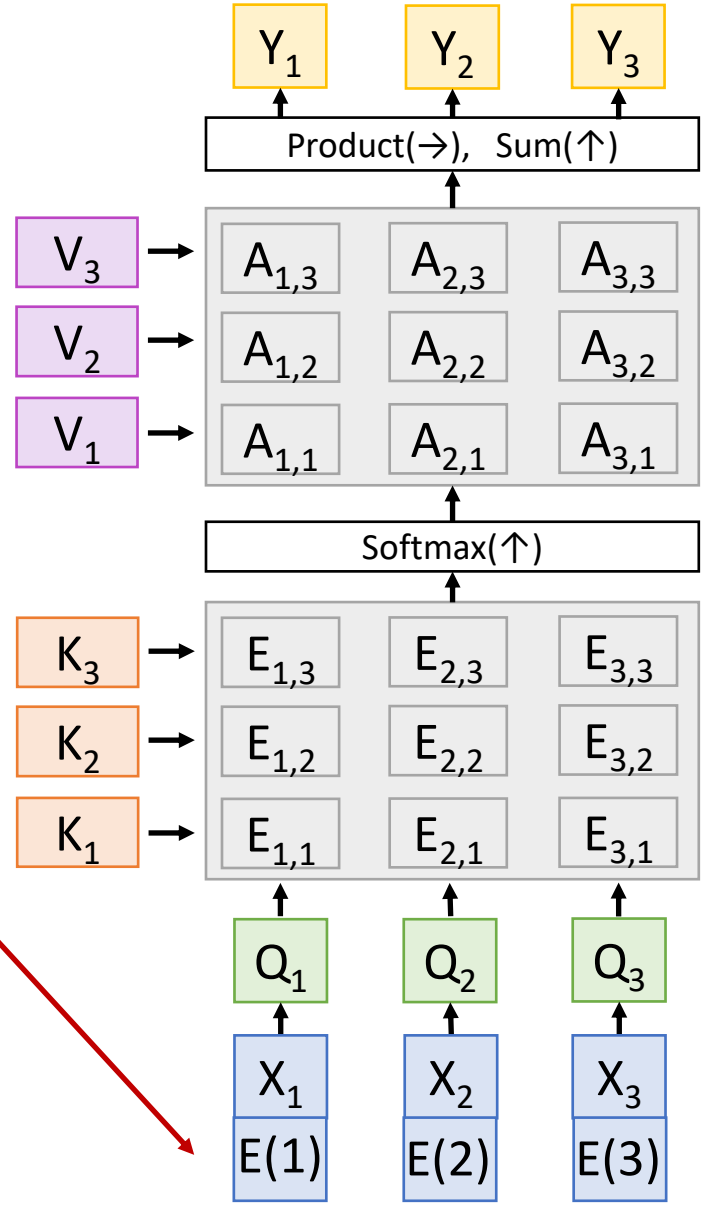
Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

Self attention doesn't "know" the order of the vectors it is processing!

In order to make processing position-aware, concatenate or add **positional encoding** to the input

E can be learned lookup table, or fixed function



Masked Self-Attention Layer

Don't let vectors "look ahead" in the sequence

Inputs:

Input vectors: X (Shape: N_X x D_X)

Key matrix: W_K (Shape: D_X x D_Q)

Value matrix: W_V (Shape: D_X x D_V)

Query matrix: W_Q (Shape: D_X x D_Q)

Computation:

Query vectors: $Q = XW_Q$

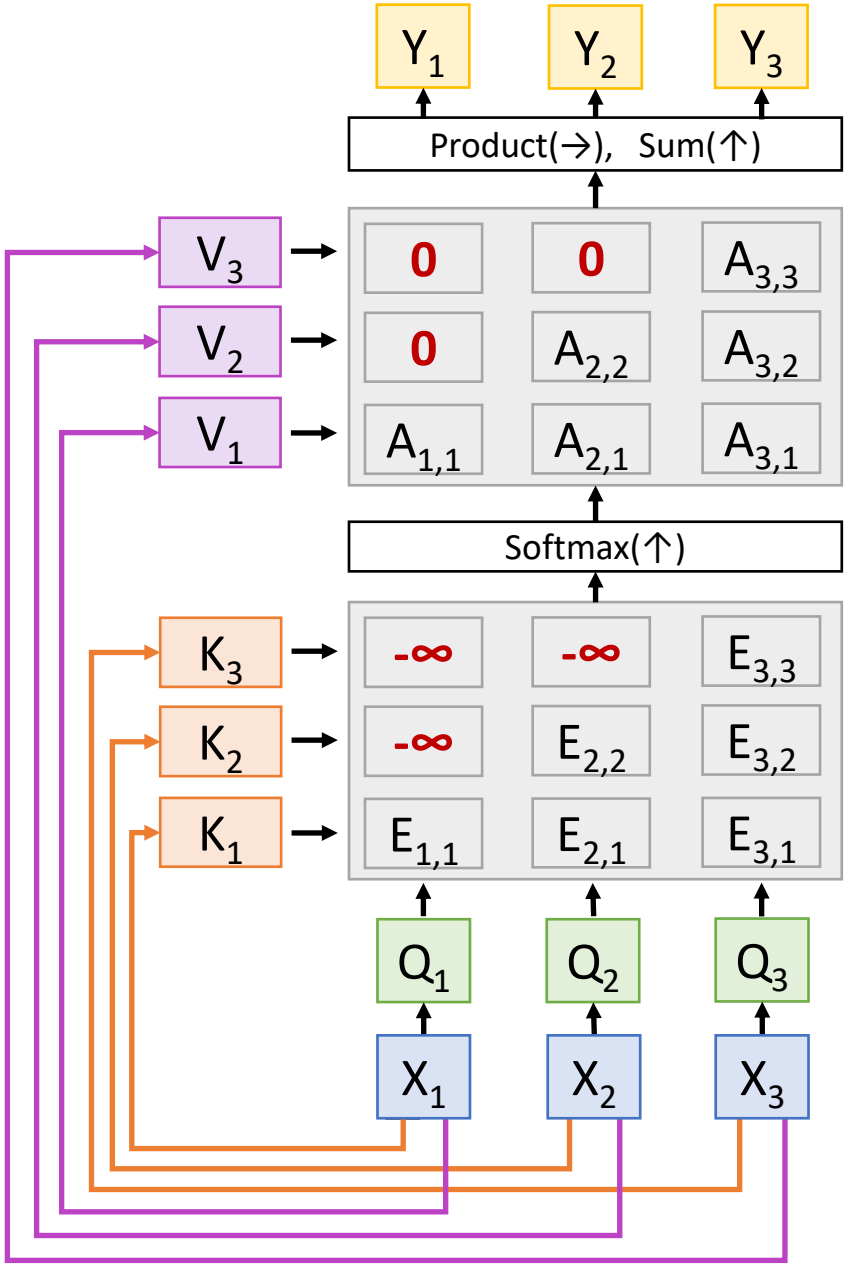
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)

Value Vectors: $V = XW_V$ (Shape: N_X x D_V)

Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$

Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)

Output vectors: Y = AV (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Masked Self-Attention Layer

Don't let vectors "look ahead" in the sequence

Used for language modeling (predict next word)

Inputs:

Input vectors: X (Shape: N_X x D_X)

Key matrix: W_K (Shape: D_X x D_Q)

Value matrix: W_V (Shape: D_X x D_V)

Query matrix: W_Q (Shape: D_X x D_Q)

Computation:

Query vectors: $Q = XW_Q$

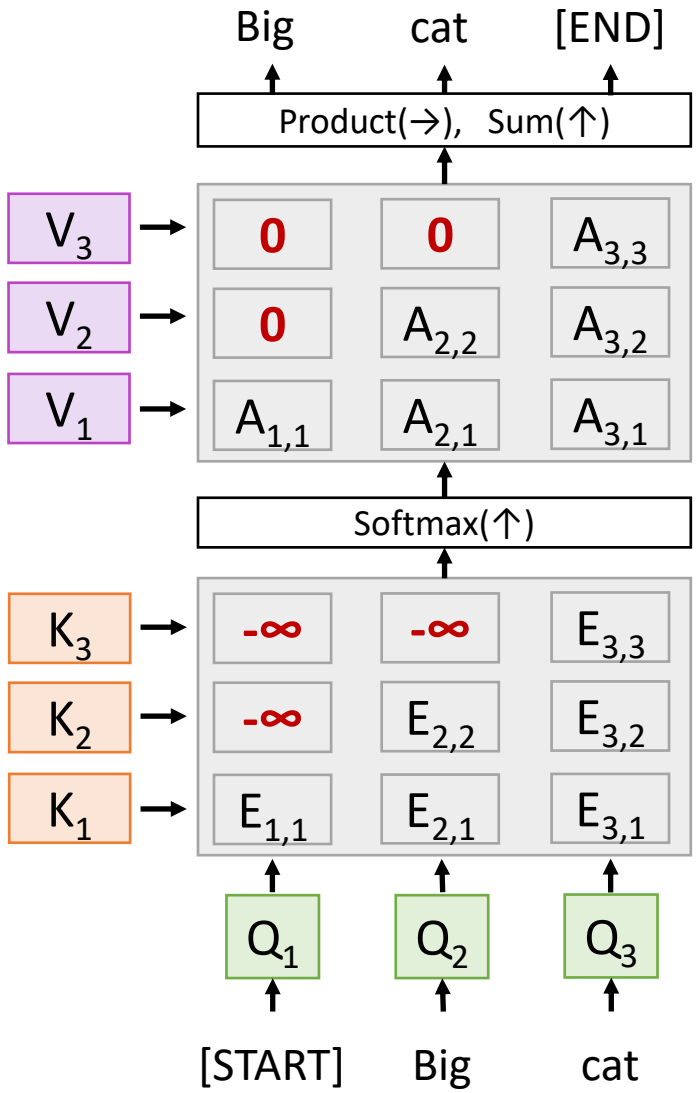
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)

Value Vectors: $V = XW_V$ (Shape: N_X x D_V)

Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$

Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)

Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Multihead Self-Attention

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Use H independent "Attention Heads" in parallel

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
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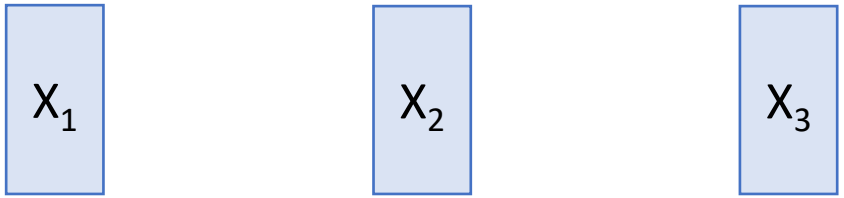

Multihead Self-Attention

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Key matrix: W_K (Shape: D_X x D_Q)
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Query matrix: W_Q (Shape: D_X x D_Q)

Use H independent "Attention Heads" in parallel

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
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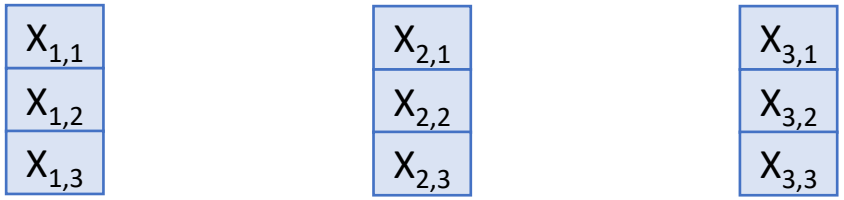
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

Split

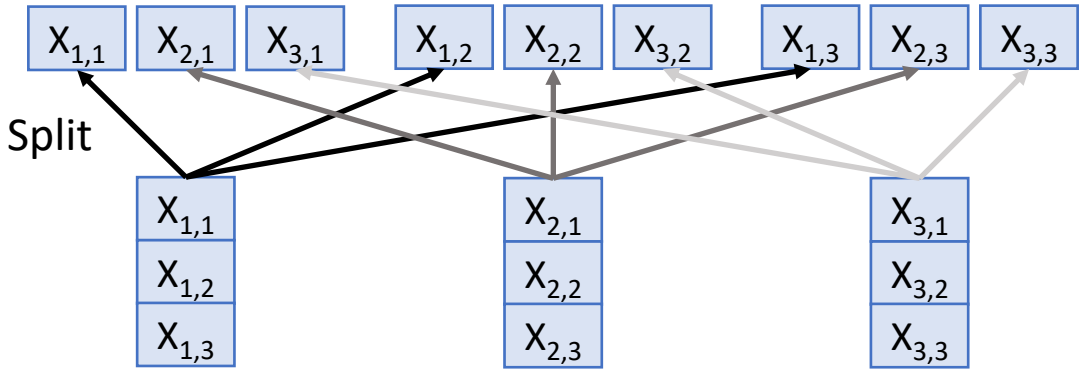


Multihead Self-Attention

Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Use H independent "Attention Heads" in parallel

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value Vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: N_X x N_X) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$



Multihead Self-Attention

Run self-attention in parallel on each set of input vectors (different weights per head)

Inputs:

Input vectors: X (Shape: $N_X \times D_X$)

Key matrix: W_K (Shape: $D_X \times D_Q$)

Value matrix: W_V (Shape: $D_X \times D_V$)

Query matrix: W_Q (Shape: $D_X \times D_Q$)

Use H independent "Attention Heads" in parallel

Computation:

Query vectors: $Q = XW_Q$

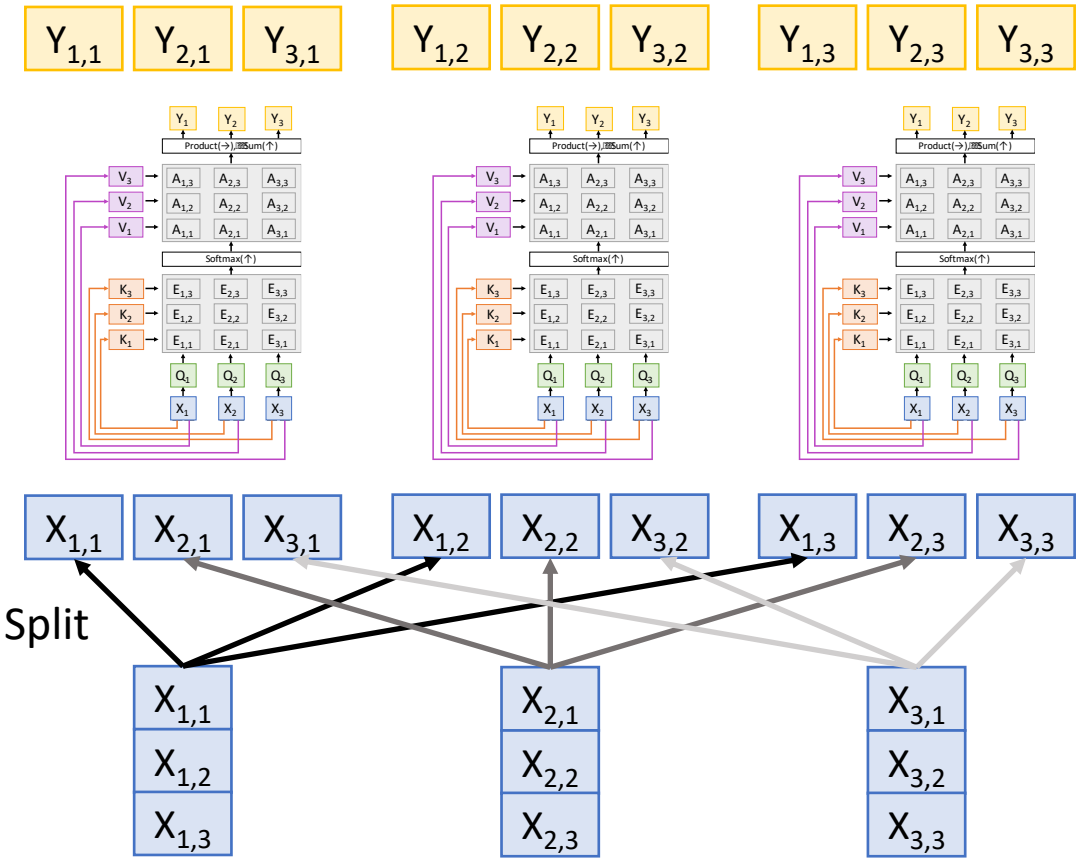
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)

Value Vectors: $V = XW_V$ (Shape: $N_X \times D_V$)

Similarities: $E = QK^T / \sqrt{D_Q}$ (Shape: $N_X \times N_X$) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$

Attention weights: $A = \text{softmax}(E, \text{dim}=1)$ (Shape: $N_X \times N_X$)

Output vectors: $Y = AV$ (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$



Multihead Self-Attention

Inputs:

Input vectors: X (Shape: $N_X \times D_X$)

Key matrix: W_K (Shape: $D_X \times D_Q$)

Value matrix: W_V (Shape: $D_X \times D_V$)

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Use H independent "Attention Heads" in parallel

Computation:

Query vectors: $Q = XW_Q$

Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)

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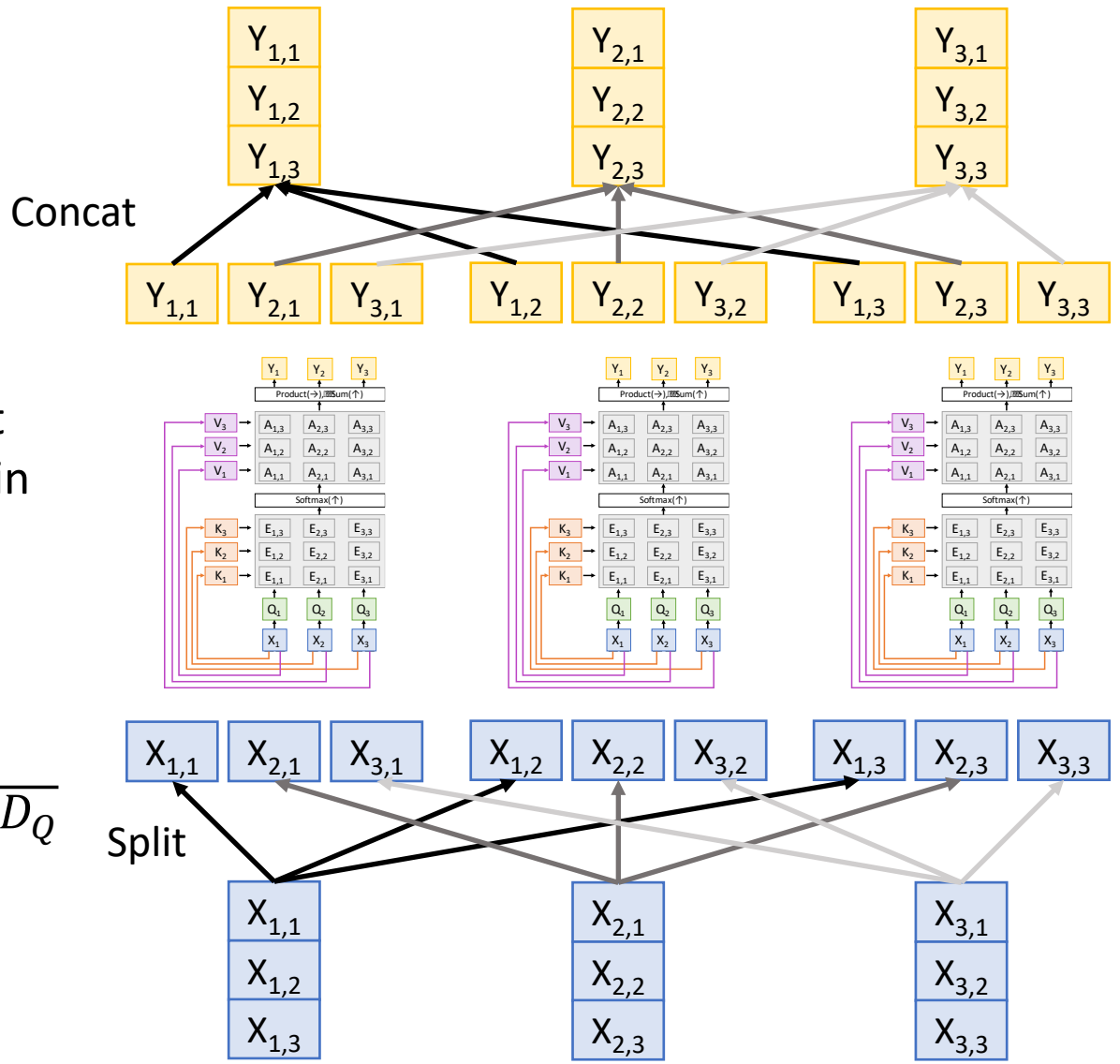

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Input vectors: X (Shape: $N_X \times D_X$)

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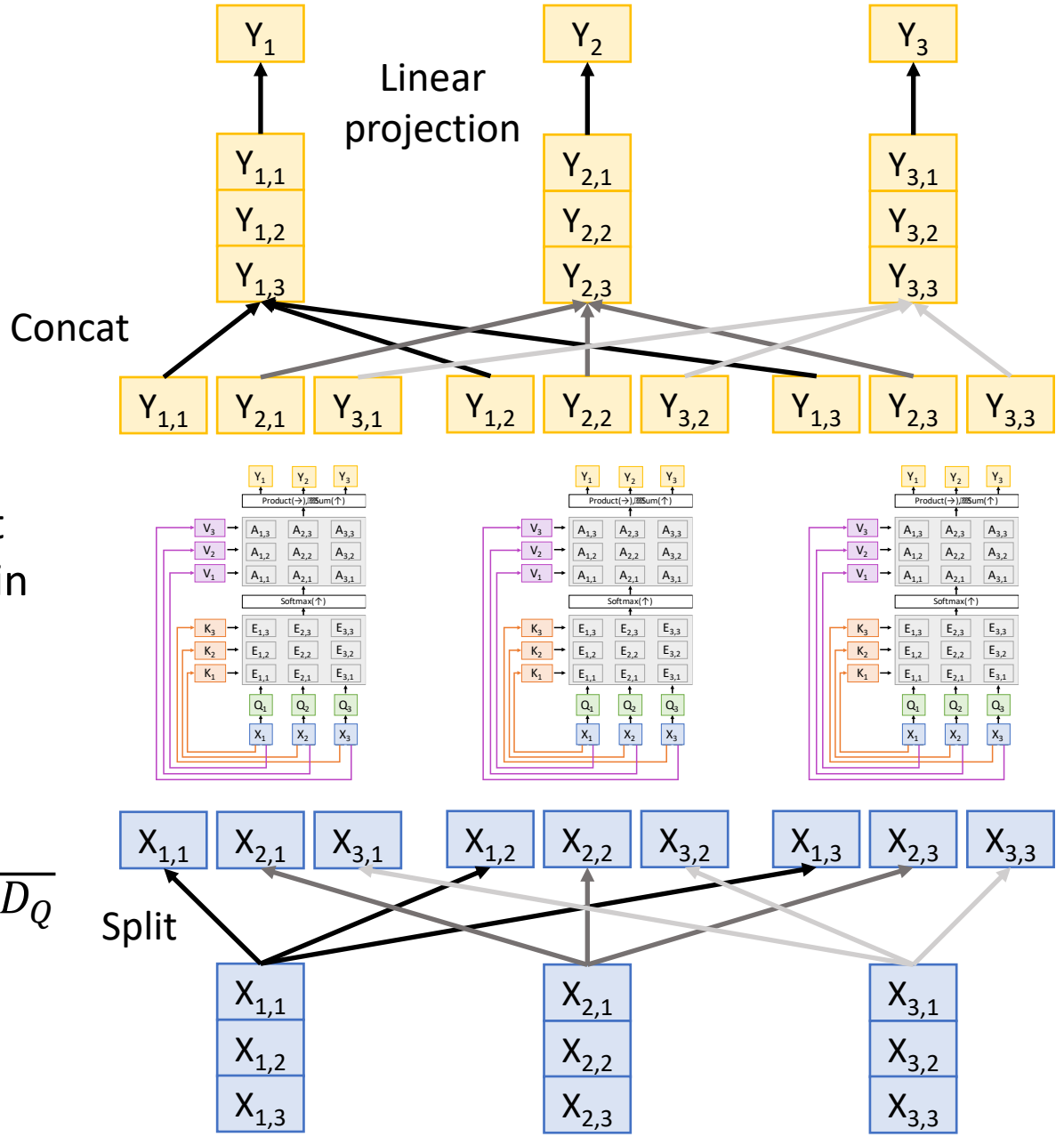


PyTorch MutiheadAttention Layer

CLASS torch.nn.MultiheadAttention(*embed_dim*, *num_heads*, *dropout=0.0*, *bias=True*, *add_bias_kv=False*, *add_zero_attn=False*, *kdim=None*, *vdim=None*, *batch_first=False*, *device=None*, *dtype=None*) [SOURCE]

Allows the model to jointly attend to information from different representation subspaces as described in the paper: Attention Is All You Need.

Multi-Head Attention is defined as:

$$\text{MultiHead}(Q, K, V) = \text{Concat}(head_1, \ldots, head_h)W^O$$

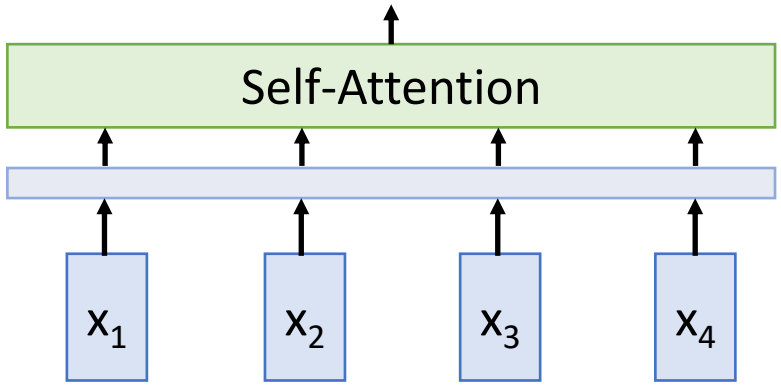
where $head_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$.

The Transformer

Vaswani et al, “Attention is all you need”, NeurIPS 2017

The Transformer

All vectors interact with each other

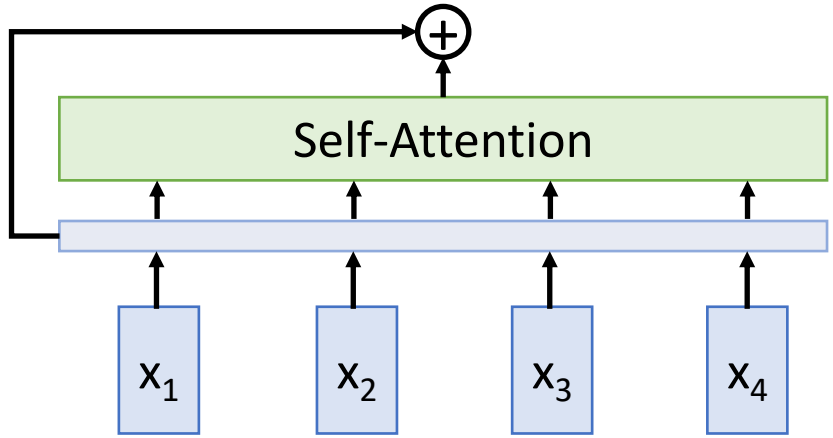


Vaswani et al, “Attention is all you need”, NeurIPS 2017

The Transformer

Residual connection

All vectors interact with each other



Vaswani et al, “Attention is all you need”, NeurIPS 2017

The Transformer

Recall **Layer Normalization**:

Given $h_1, \ldots, h_N$ (Shape: D)

scale: γ (Shape: D)

shift: β (Shape: D)

$\mu_i = (\sum_j h_{i,j})/D$ (scalar)

$\sigma_i = (\sum_j (h_{i,j} - \mu_i)^2/D)^{1/2}$ (scalar)

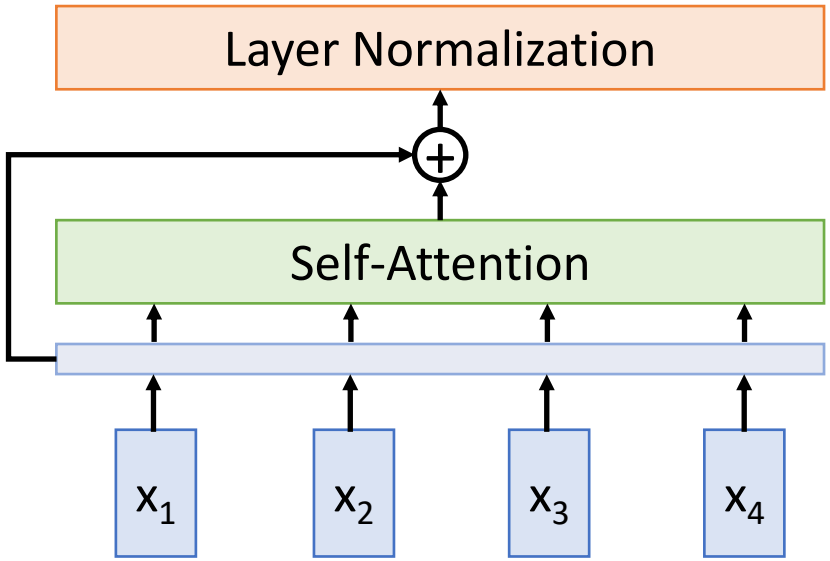
$z_i = (h_i - \mu_i) / \sigma_i$

$y_i = \gamma * z_i + \beta$

Ba et al, 2016

Residual connection

All vectors interact with each other



Vaswani et al, "Attention is all you need", NeurIPS 2017

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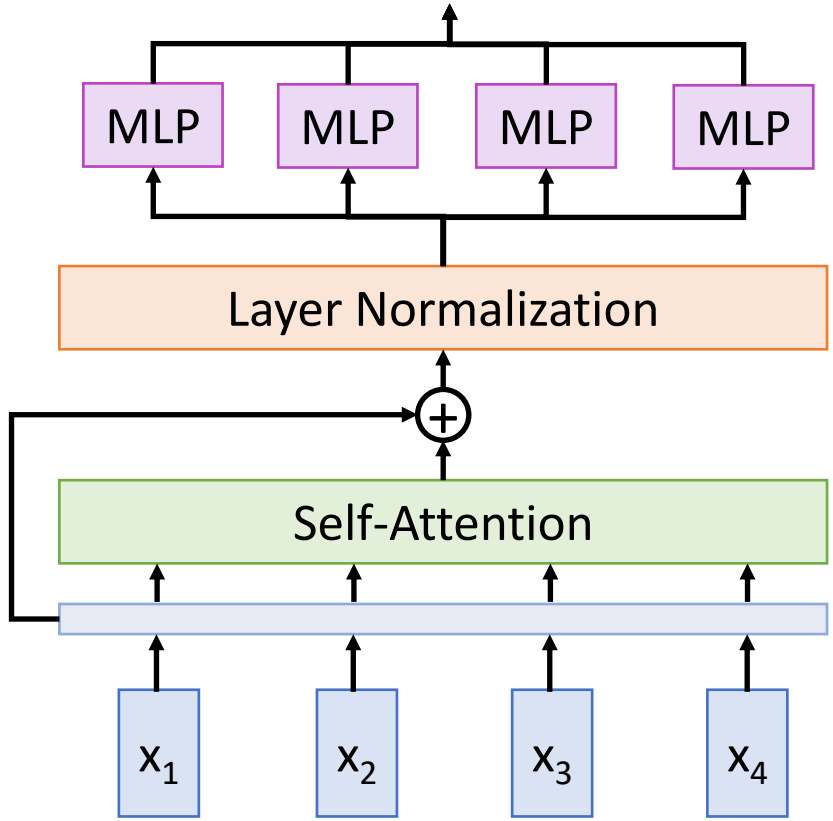
Ba et al, 2016

MLP independently on each vector

Residual connection

All vectors interact with each other



Vaswani et al, "Attention is all you need", NeurIPS 2017

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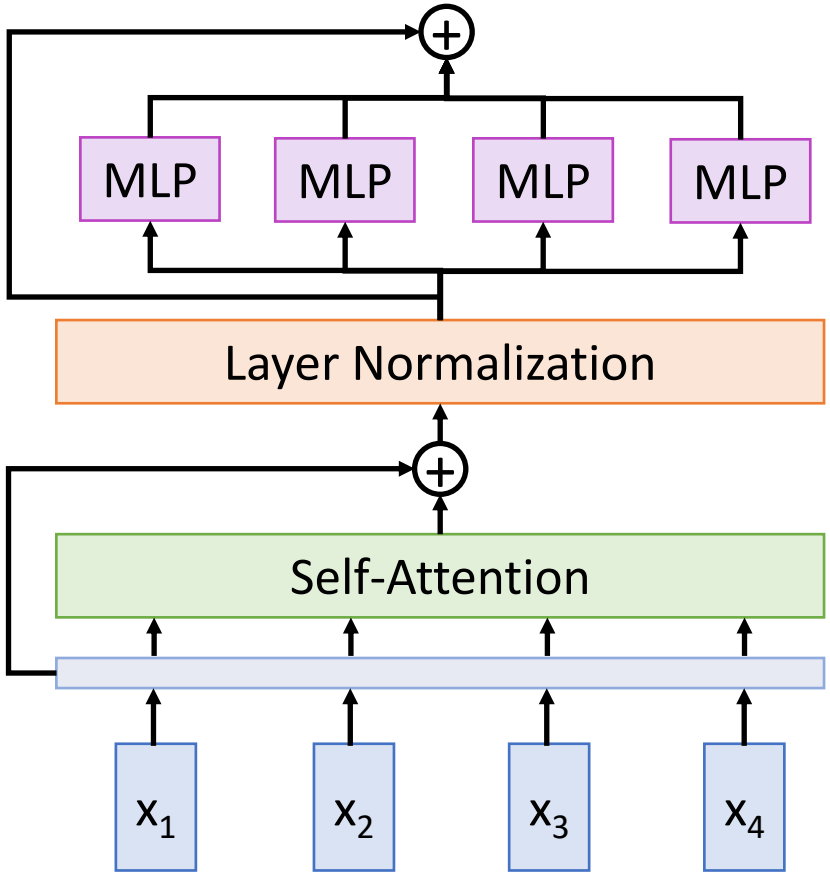
Ba et al, 2016

Residual connection

MLP independently on each vector

Residual connection

All vectors interact with each other



Vaswani et al, "Attention is all you need", NeurIPS 2017

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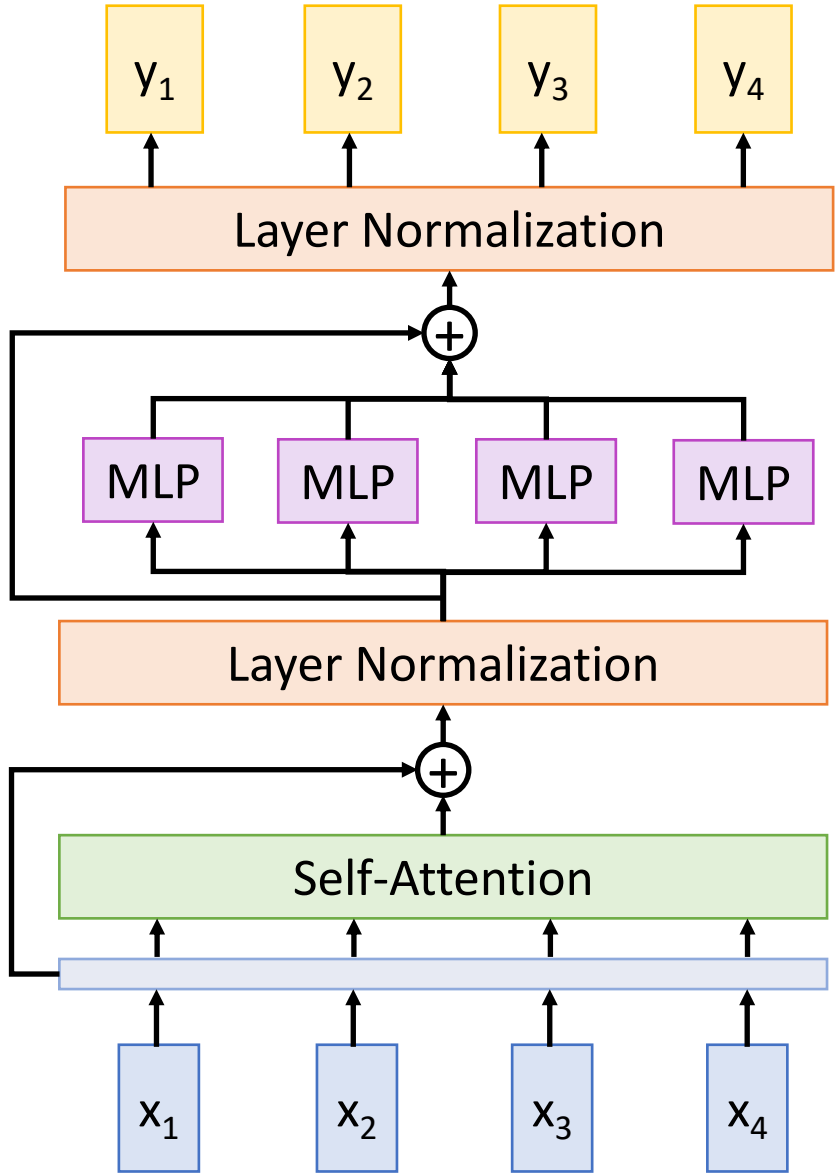


Vaswani et al, "Attention is all you need", NeurIPS 2017

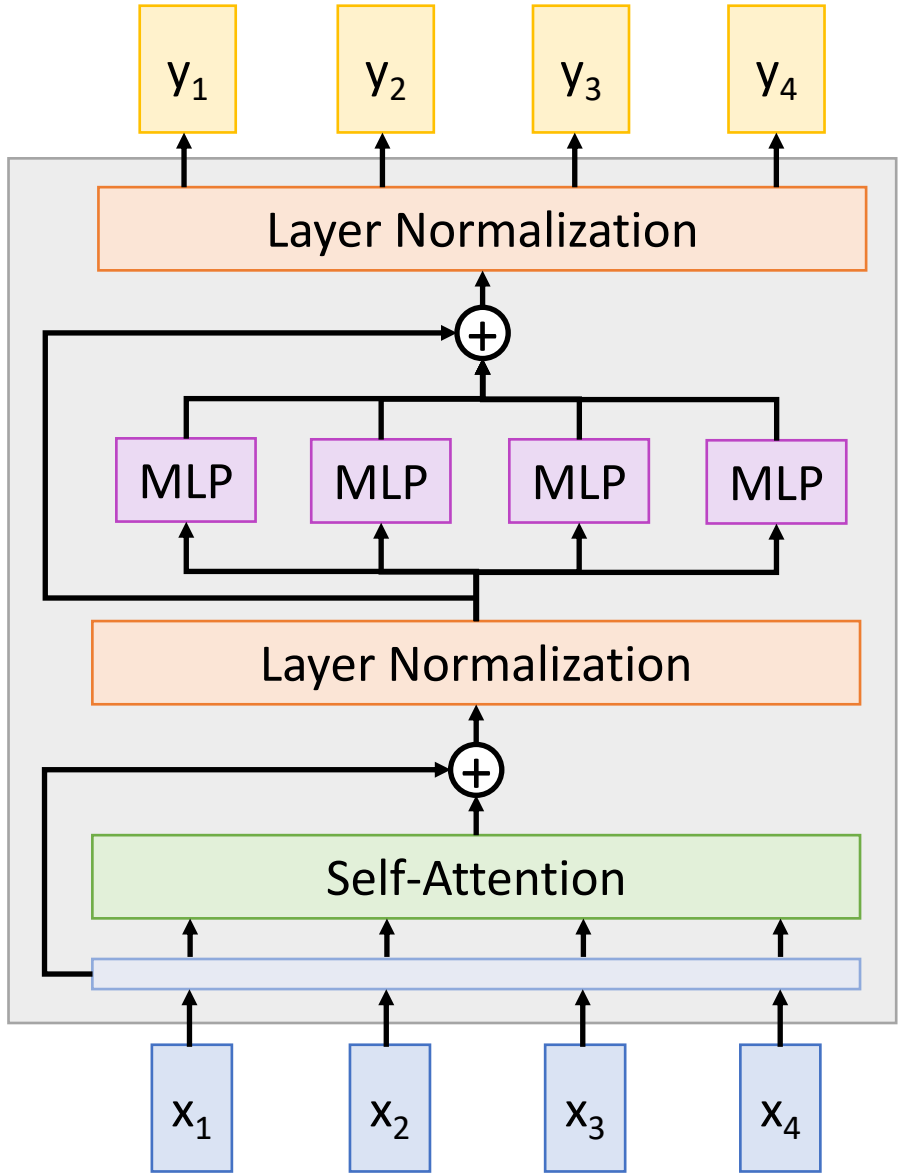
The Transformer

Transformer Block:
Input: Set of vectors x
Output: Set of vectors y

Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

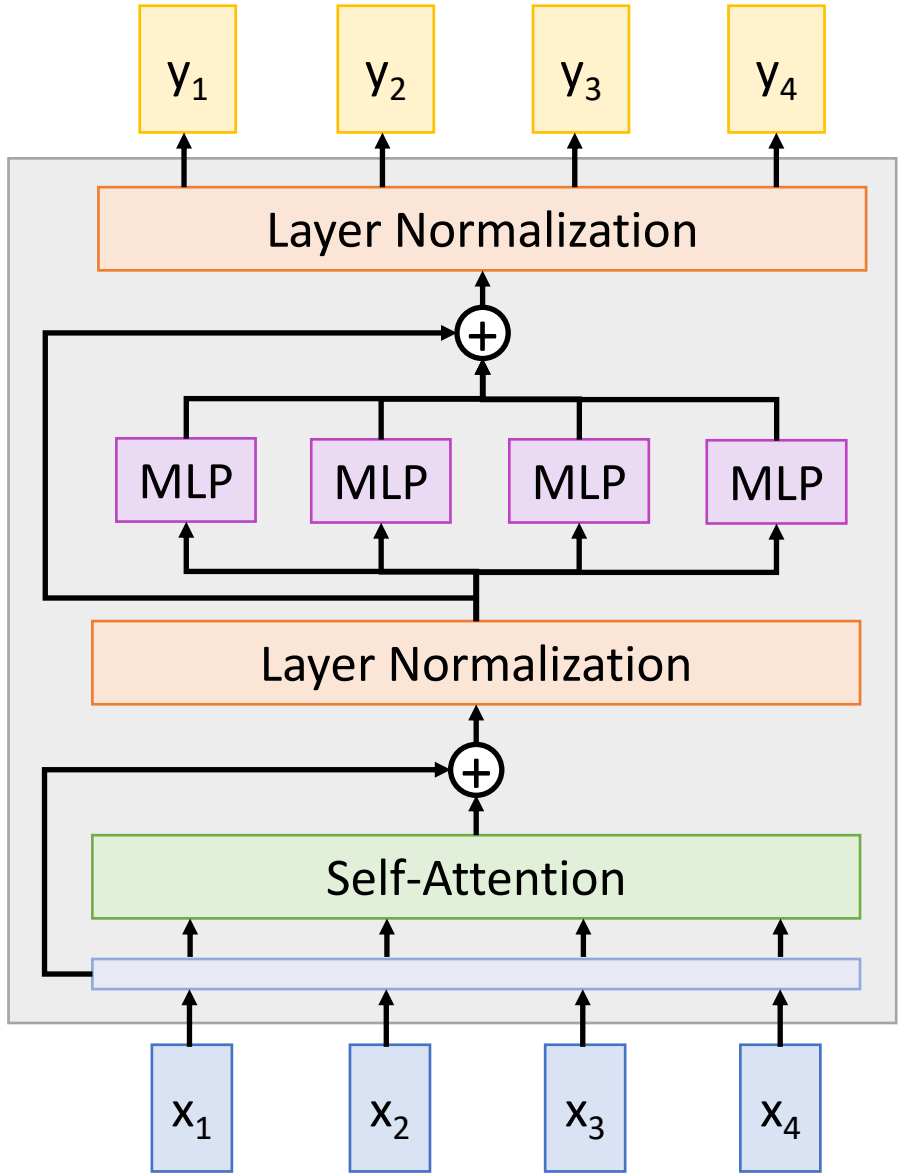
Highly scalable, highly parallelizable



Vaswani et al, "Attention is all you need", NeurIPS 2017

Post-Norm Transformer

Layer normalization is **after** residual connections

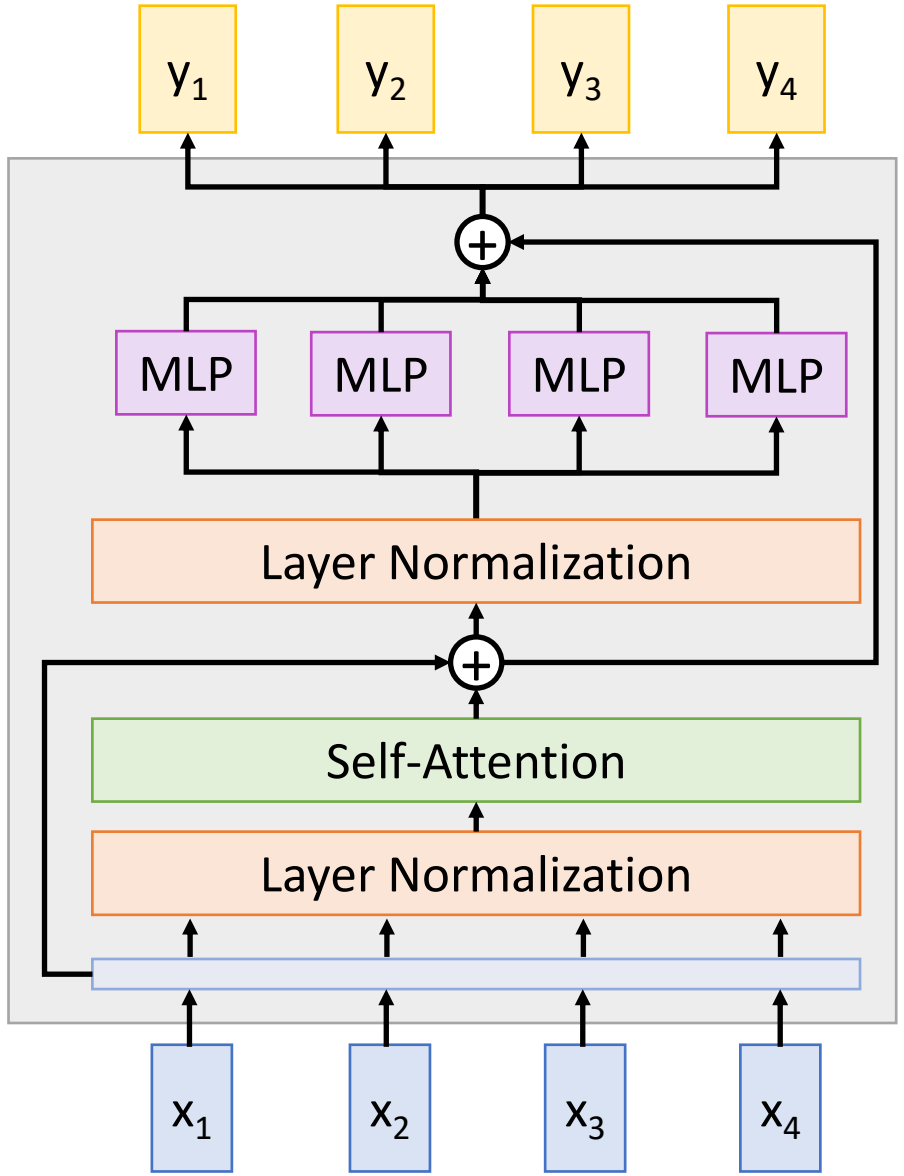


Vaswani et al, "Attention is all you need", NeurIPS 2017

Pre-Norm Transformer

Layer normalization is **inside** residual connections

Gives more stable training, commonly used in practice



Baevski & Auli, "Adaptive Input Representations for Neural Language Modeling", arXiv 2018

The Transformer

Transformer Block:
Input: Set of vectors x
Output: Set of vectors y

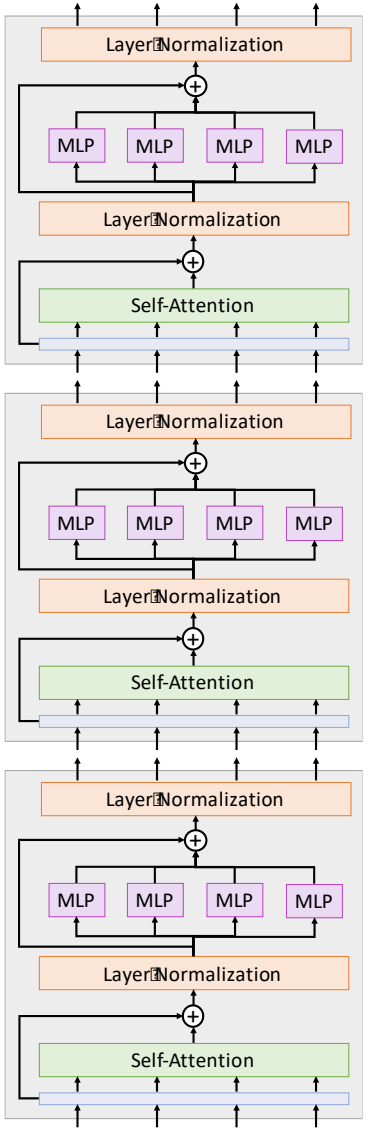
Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable

A **Transformer** is a sequence of transformer blocks

Vaswani et al:
12 blocks, D_Q=512, 6 heads



Vaswani et al, "Attention is all you need", NeurIPS 2017

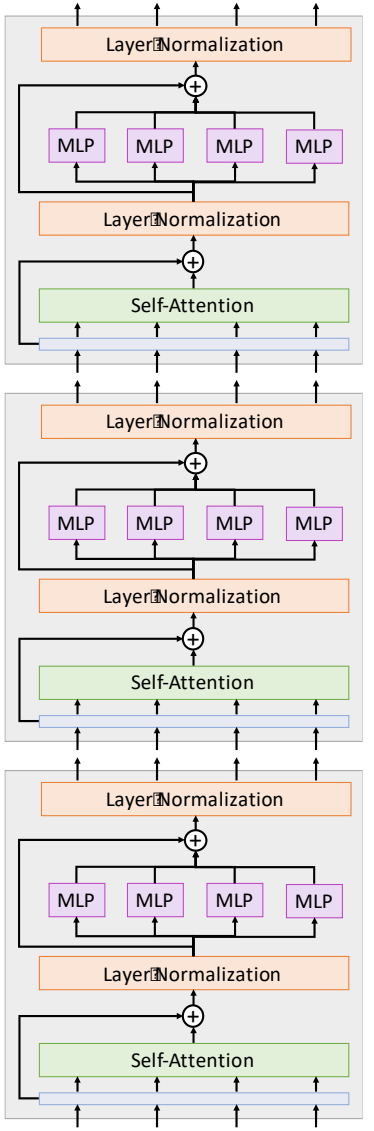
The Transformer: Transfer Learning

"ImageNet Moment for Natural Language Processing"

Pre-training:
Download a lot of text from the internet

Train a giant Transformer model for language modeling

Fine-tuning:
Fine-tune the Transformer on your own NLP task



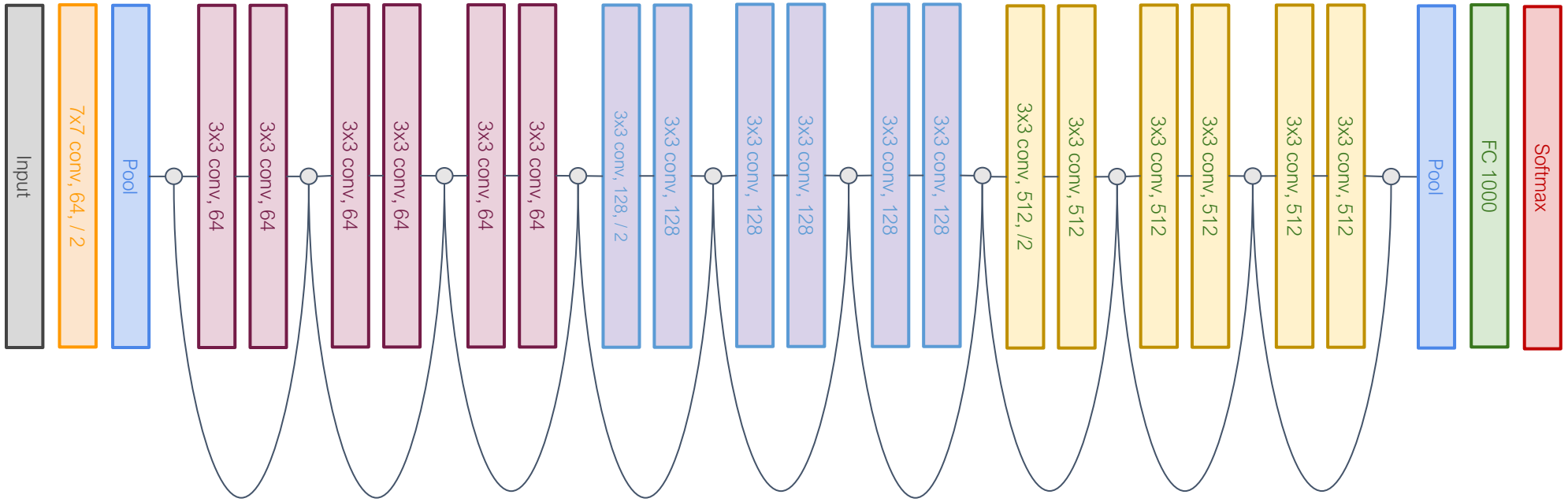
Devlin et al, "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding", EMNLP 2018

Outline

- Recurrent Neural Networks
- Attention and Transformers
- Vision Transformers

Idea #1: Add attention to existing CNNs

Start from standard CNN architecture (e.g., ResNet)



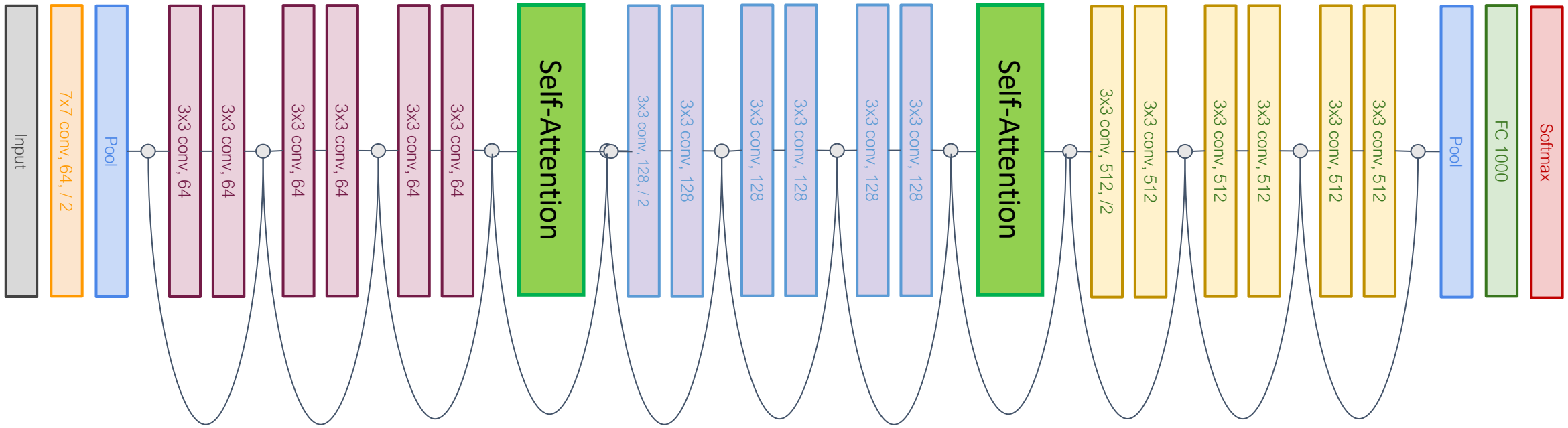
Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018
Wang et al, "Non-local Neural Networks", CVPR 2018

Idea #1: Add attention to existing CNNs

Model is still a CNN!
Can we replace convolution entirely?

Start from standard CNN architecture (e.g., ResNet)

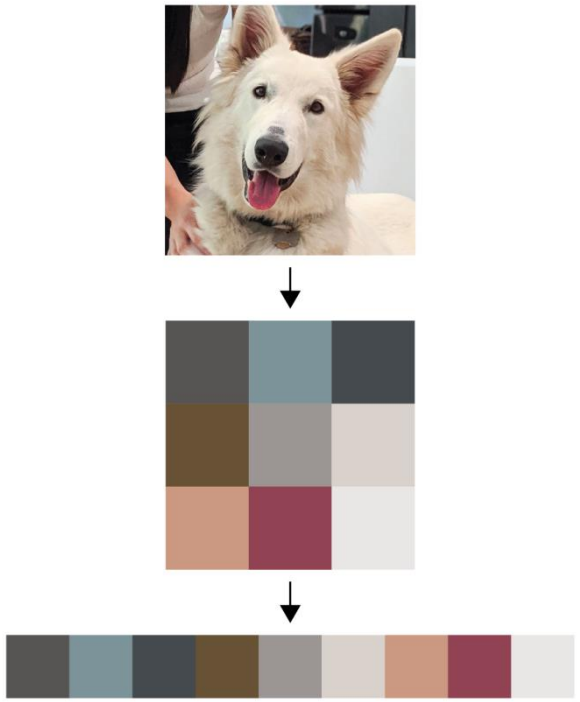
Add Self-Attention blocks between existing ResNet blocks

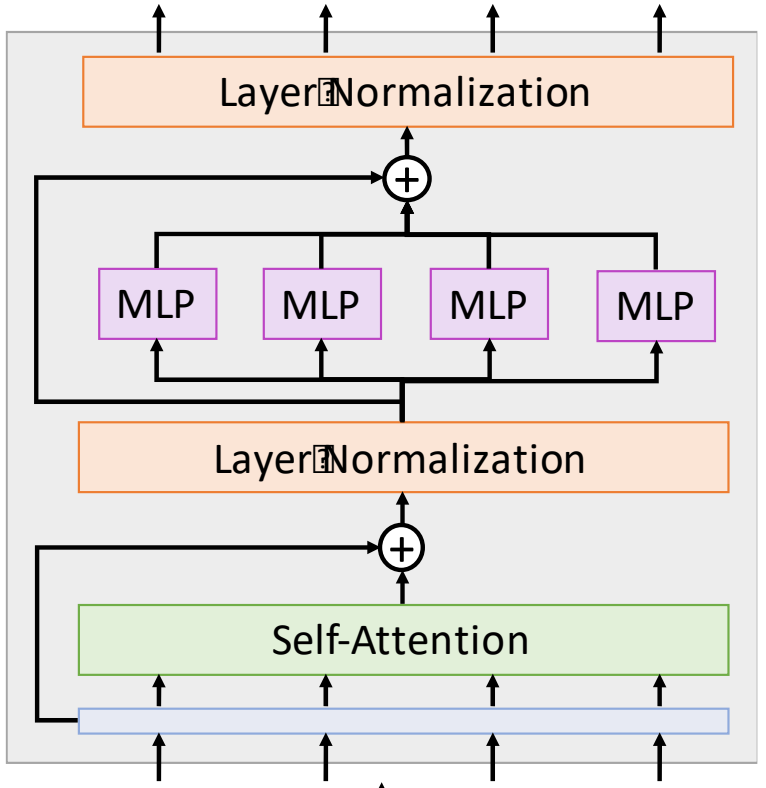


Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018
Wang et al, "Non-local Neural Networks", CVPR 2018

Idea #2: Standard Transformer on Pixels

Treat an image as a set of pixel values





Feed as input to standard Transformer

Problem: Memory use!

R x R image needs R^4 elements per attention matrix

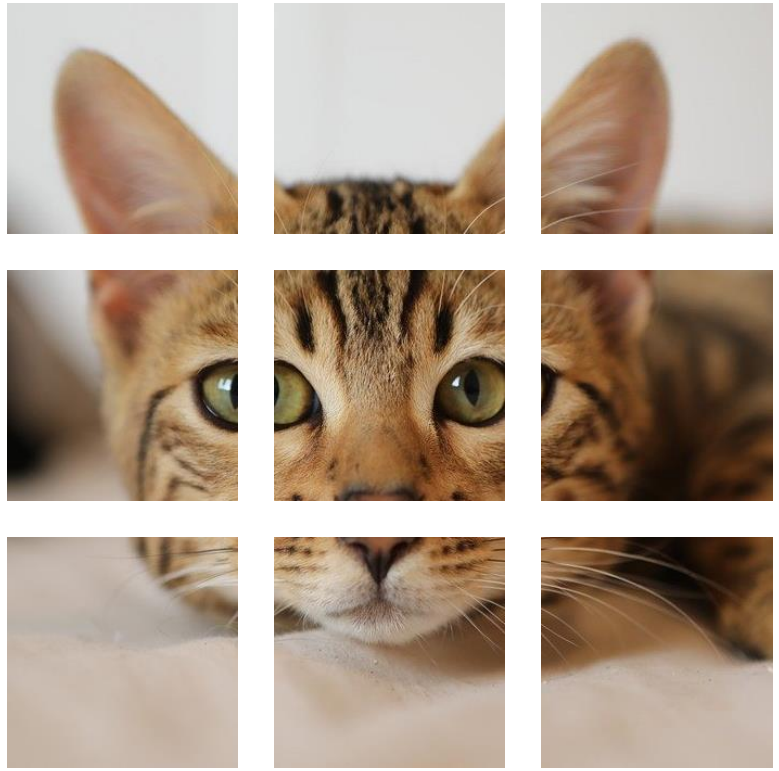
R=128, 48 layers, 16 heads per layer takes 768GB of memory for attention matrices for a single example…

Chen et al, “Generative Pretraining from Pixels”, ICML 2020

Idea #3: Standard Transformer on Patches

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Idea #3: Standard Transformer on Patches



Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Idea #3: Standard Transformer on Patches

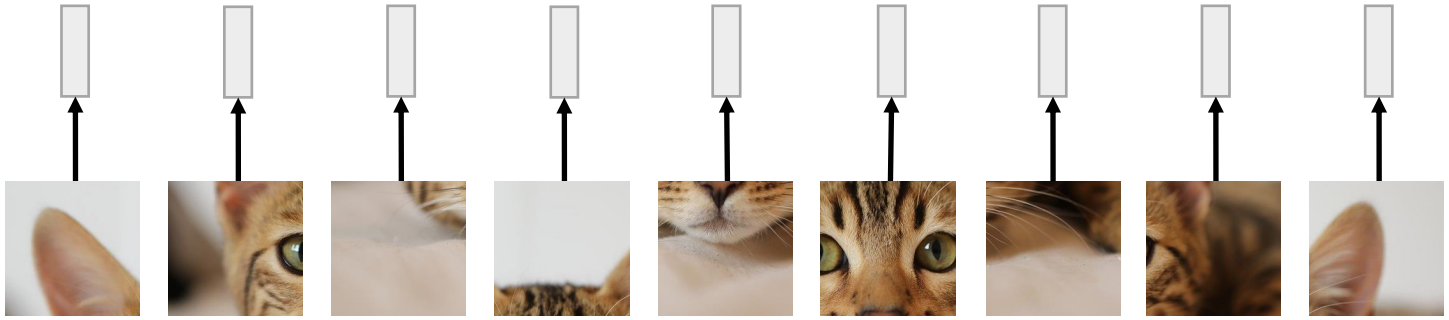
N input patches, each of shape 3x16x16

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Idea #3: Standard Transformer on Patches

Linear projection to D-dimensional vector

N input patches, each of shape 3x16x16



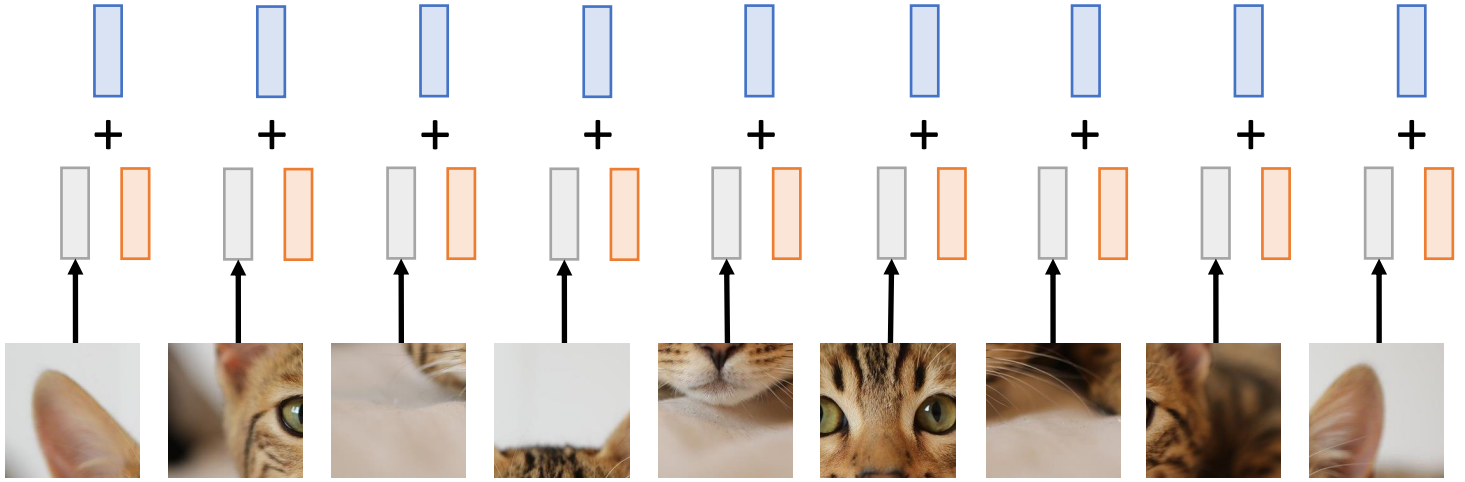
Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Idea #3: Standard Transformer on Patches

Add positional embedding: learned D-dim vector per position

Linear projection to D-dimensional vector

N input patches, each of shape 3x16x16



Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Idea #3: Standard Transformer on Patches

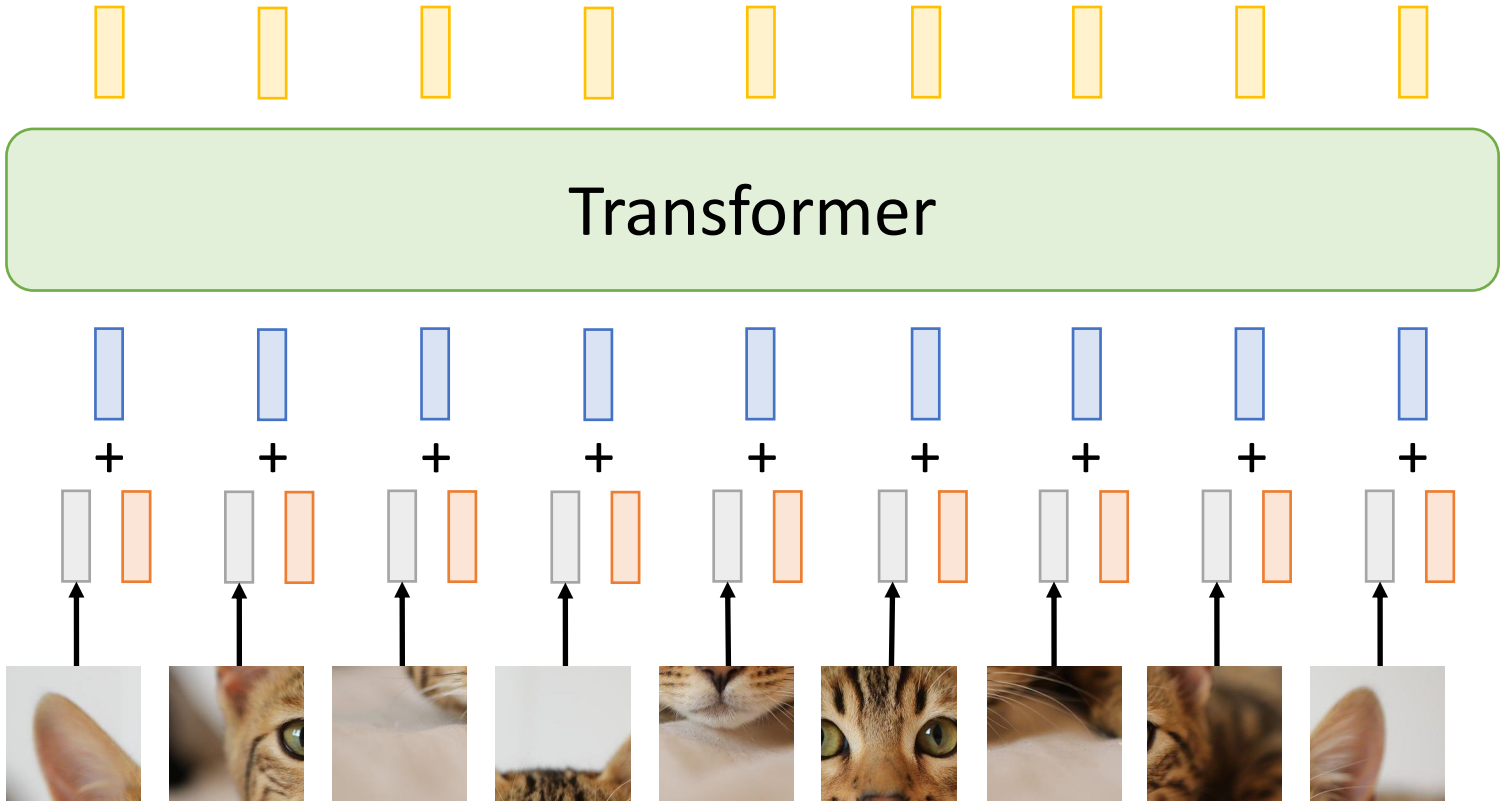
Output vectors

Exact same as NLP Transformer!

Add positional embedding: learned D-dim vector per position

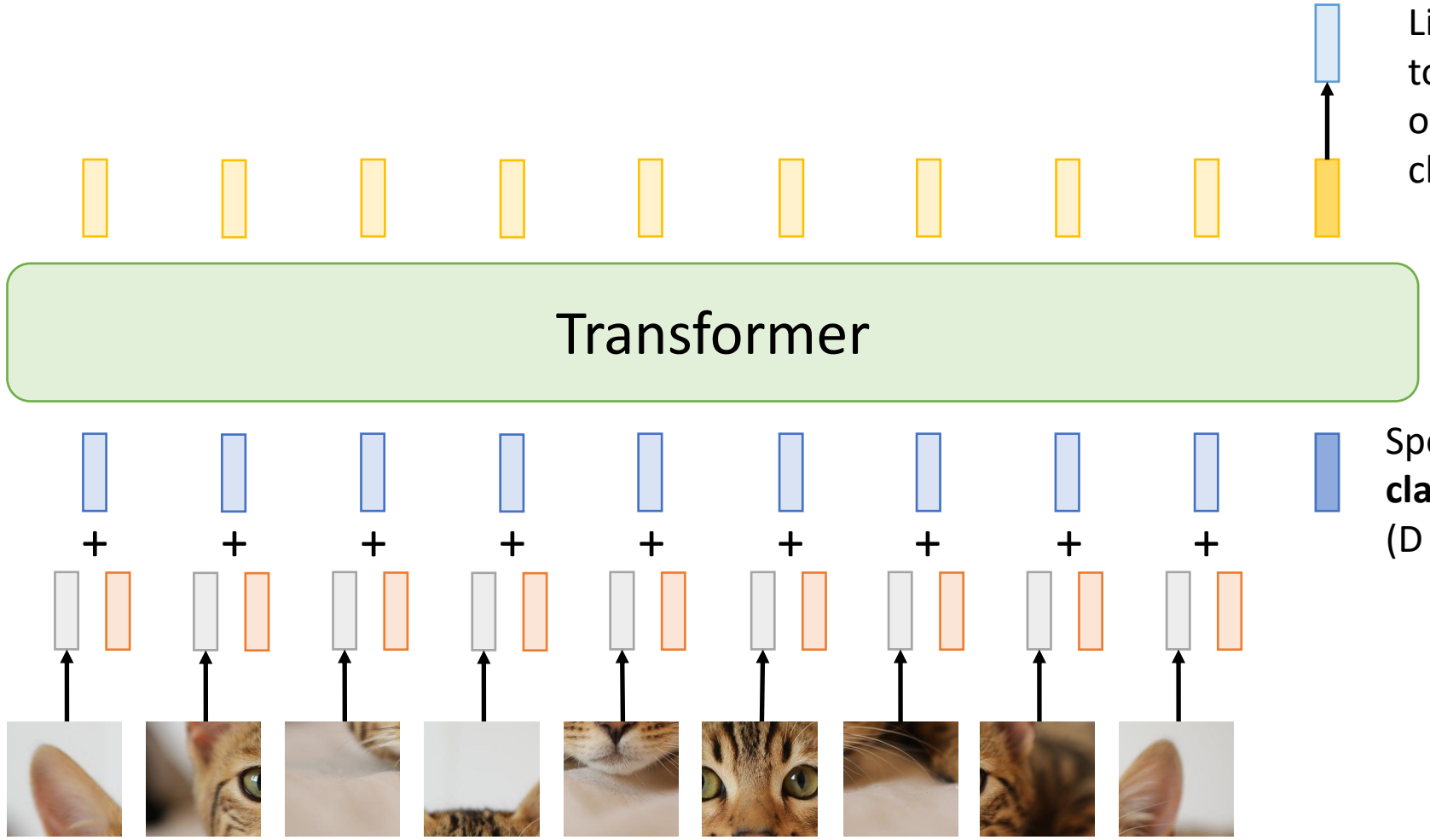
Linear projection to D-dimensional vector

N input patches, each of shape 3x16x16



Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Idea #3: Standard Transformer on Patches



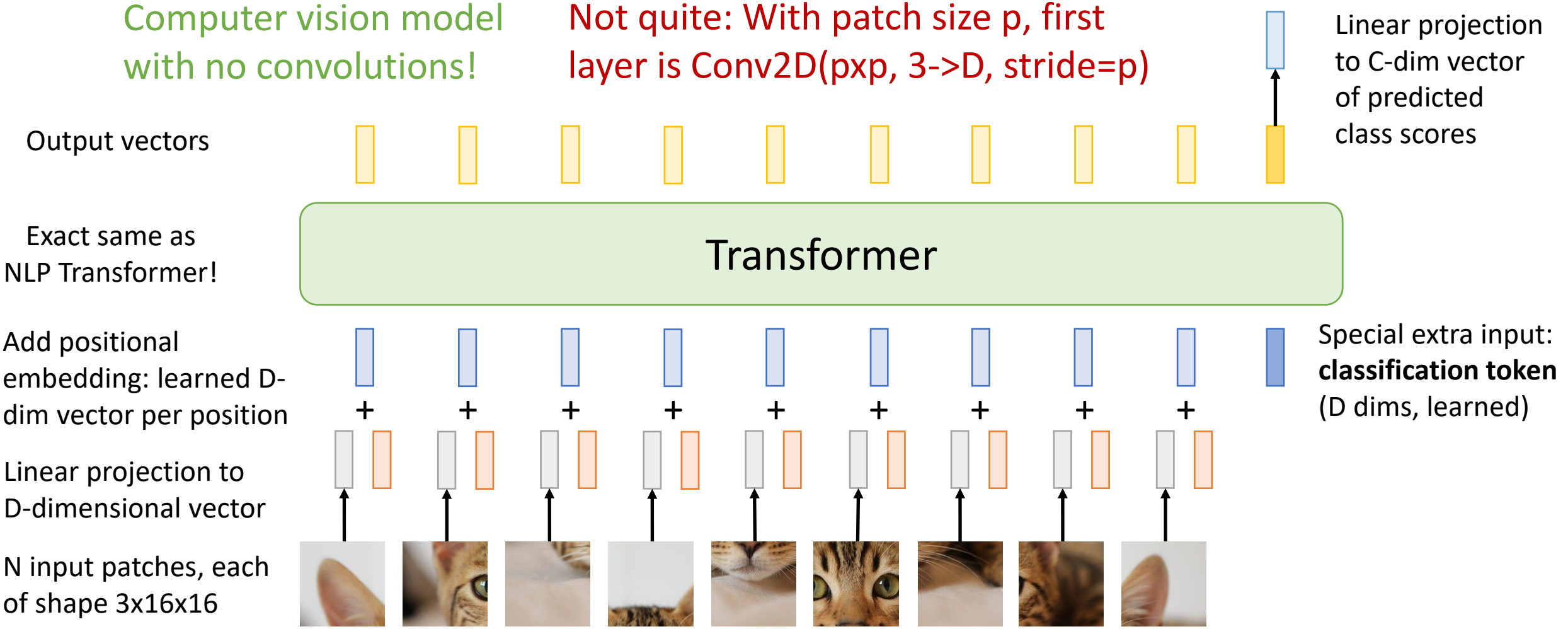
Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Cat image is free for commercial use under a Pixabay license

Vision Transformer (ViT)

Computer vision model with no convolutions!

Not quite: With patch size p, first layer is Conv2D(pxp, 3->D, stride=p)

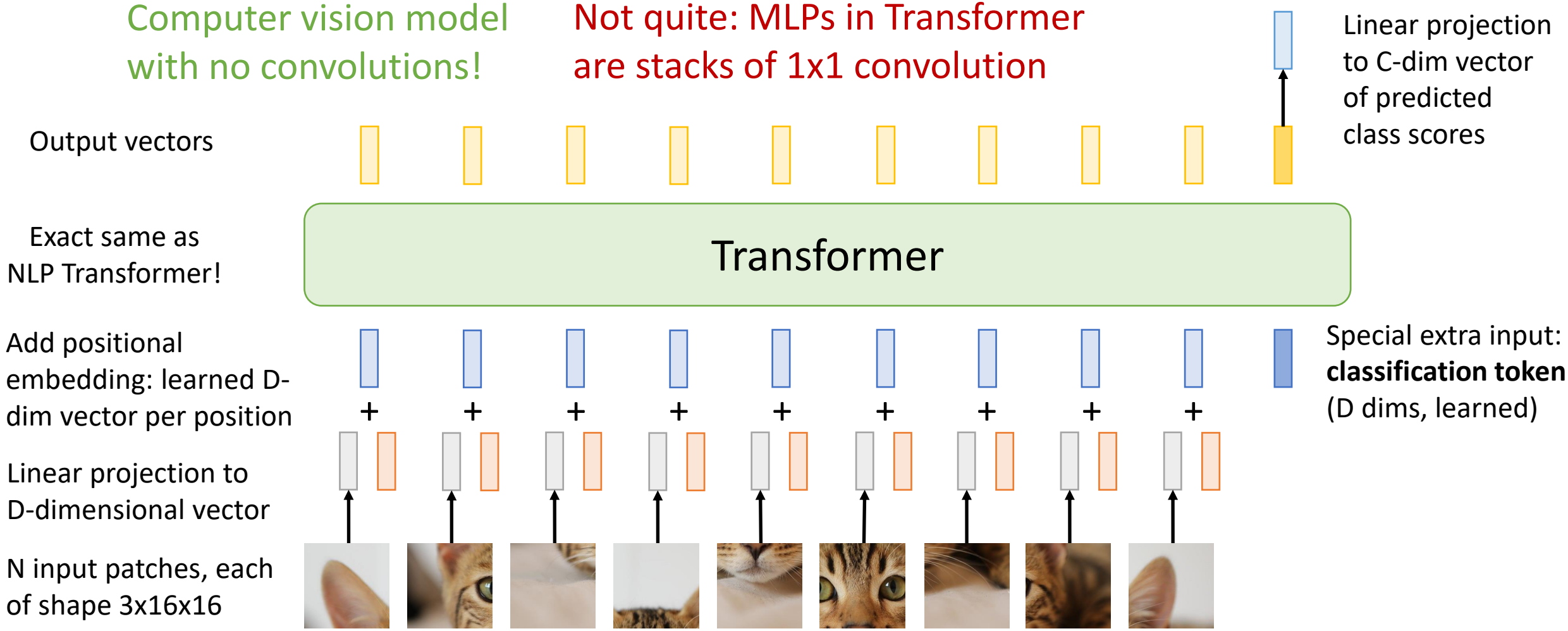


Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ICLR 2021

Vision Transformer (ViT)

Computer vision model with no convolutions!

Not quite: MLPs in Transformer are stacks of 1x1 convolution



Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

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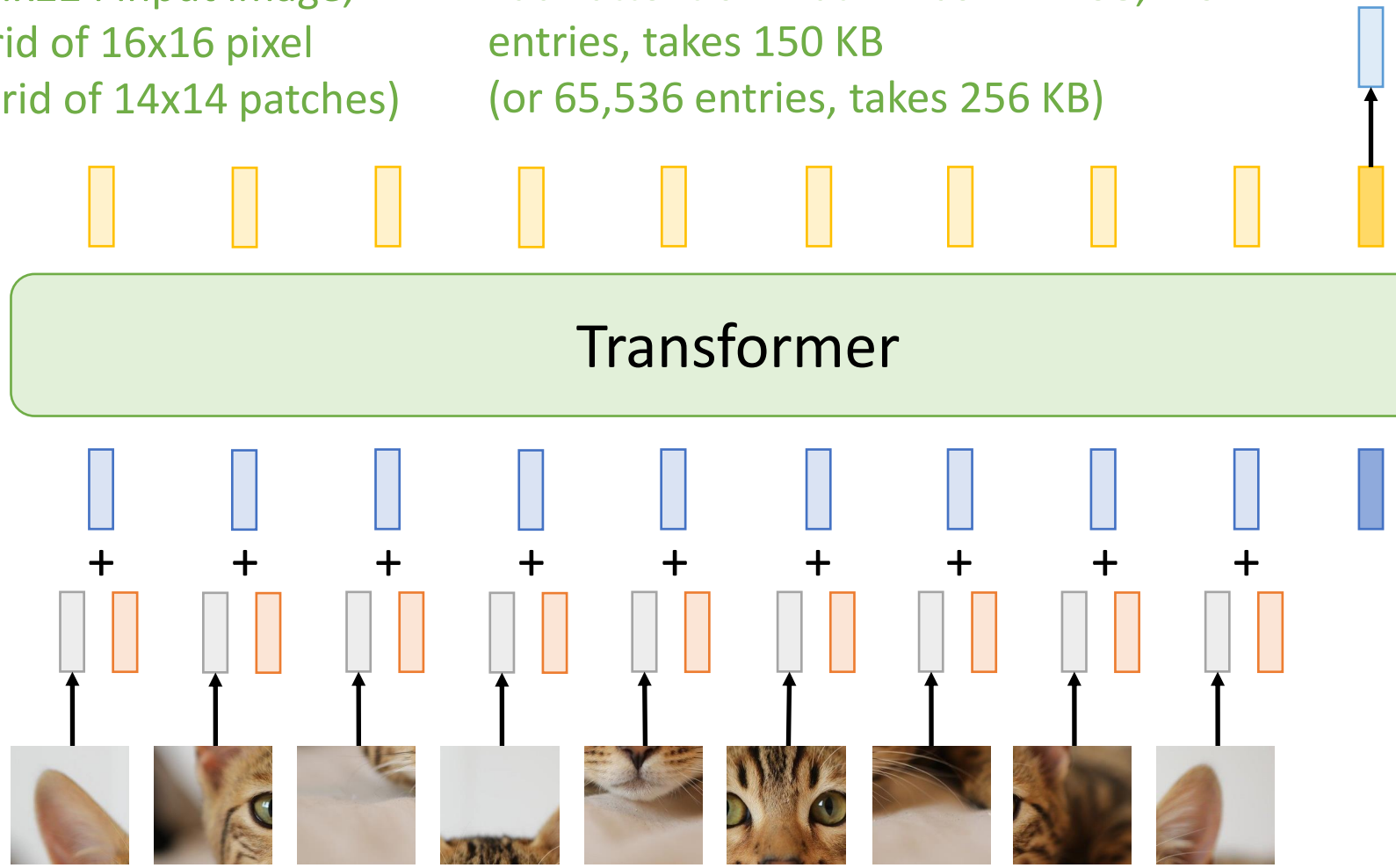
Vision Transformer (ViT)

In practice: take 224x224 input image, divide into 14x14 grid of 16x16 pixel patches (or 16x16 grid of 14x14 patches)

Each attention matrix has $14^4 = 38{,}416$ entries, takes 150 KB (or 65,536 entries, takes 256 KB)



Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ICLR 2021

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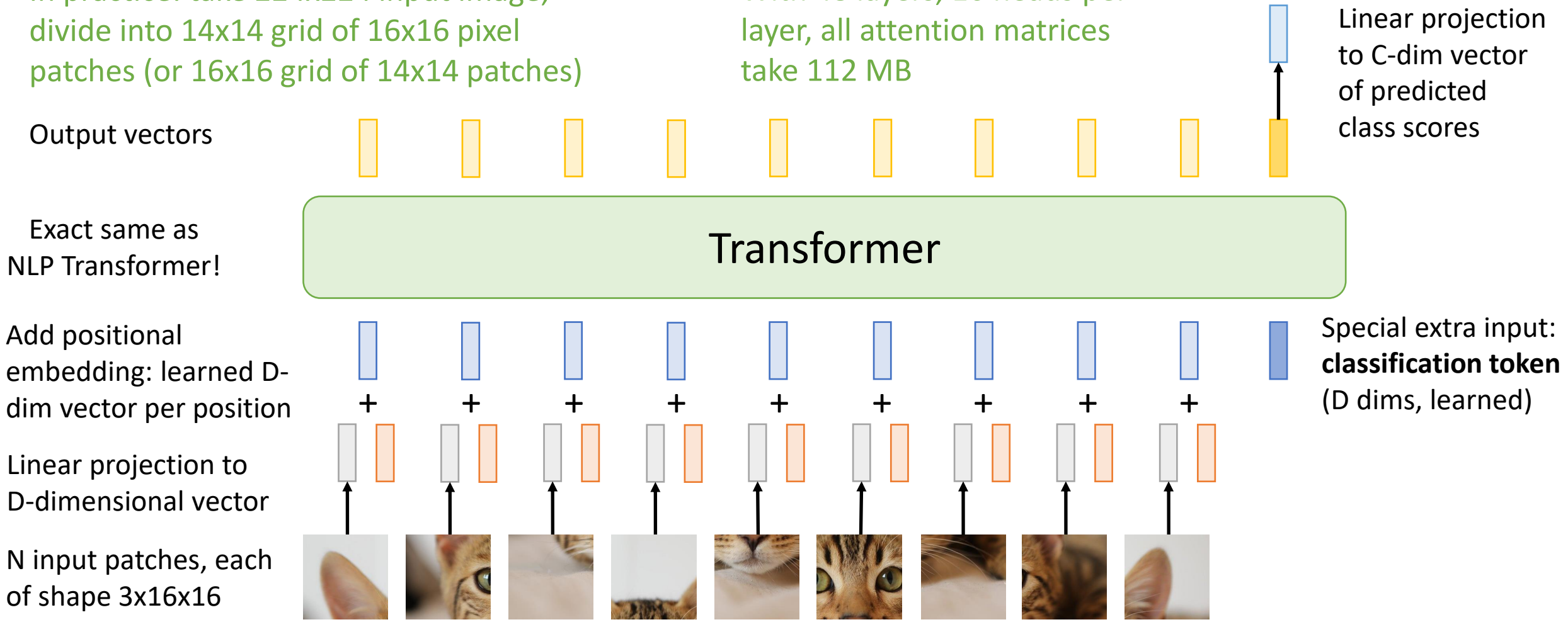
Vision Transformer (ViT)

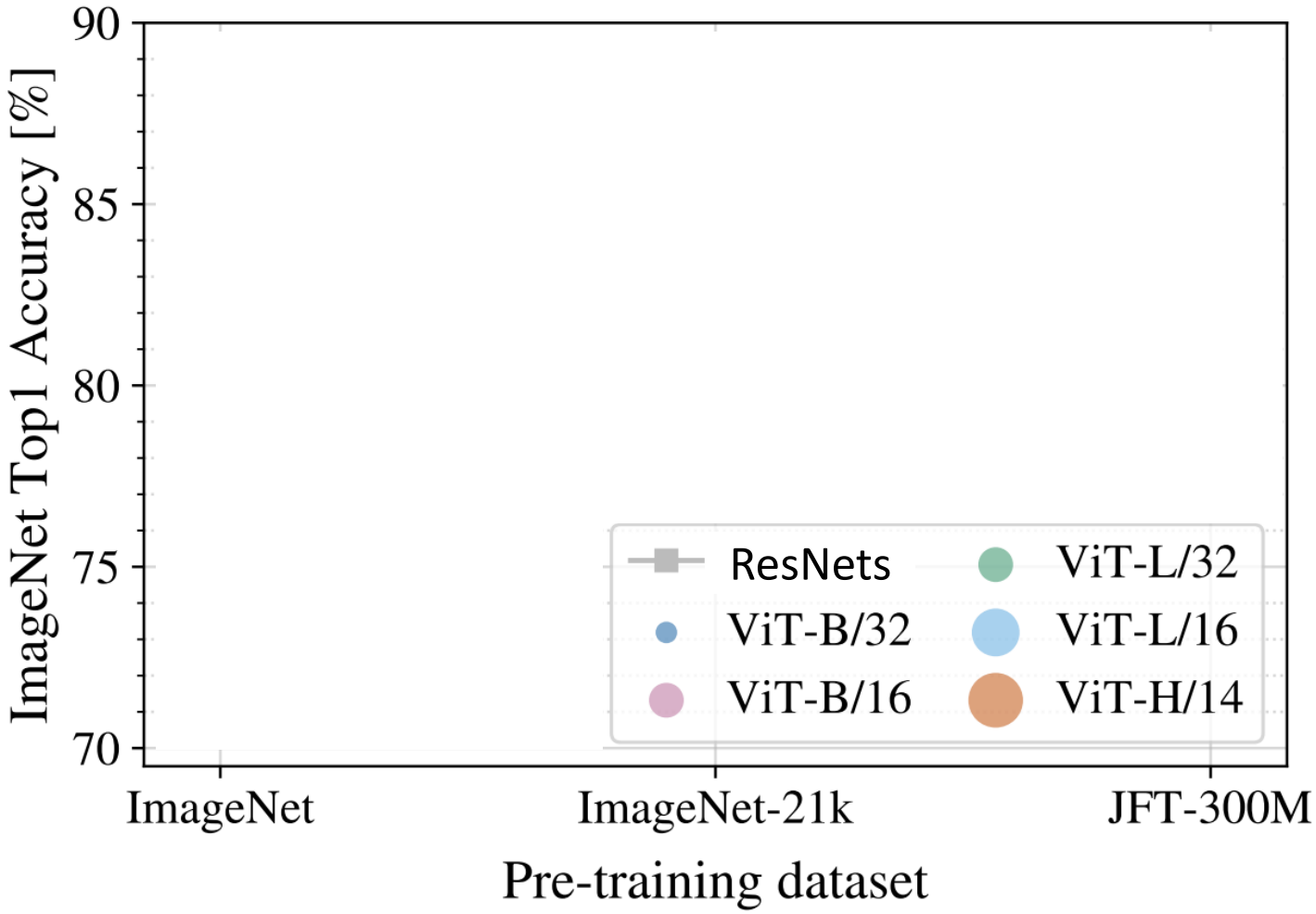
In practice: take 224x224 input image, divide into 14x14 grid of 16x16 pixel patches (or 16x16 grid of 14x14 patches)

With 48 layers, 16 heads per layer, all attention matrices take 112 MB



Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Vision Transformer (ViT) vs. ResNets



B = Base
L = Large
H = Huge

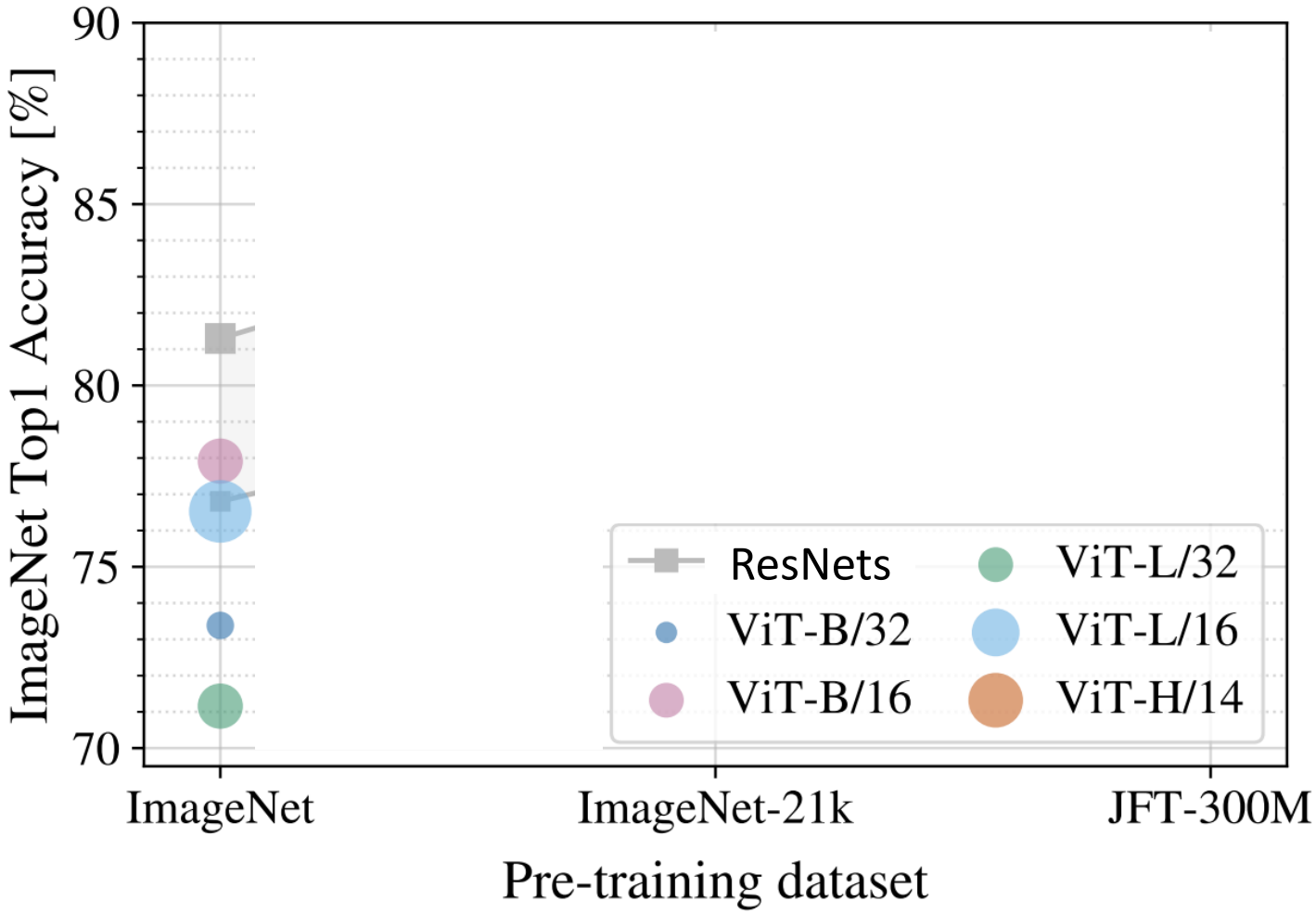
/32, /16, /14 is patch size; smaller patch size is a bigger model (more patches)

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Vision Transformer (ViT) vs. ResNets

Recall: ImageNet dataset has 1k categories, 1.2M images

When trained on ImageNet, ViT models perform worse than ResNets



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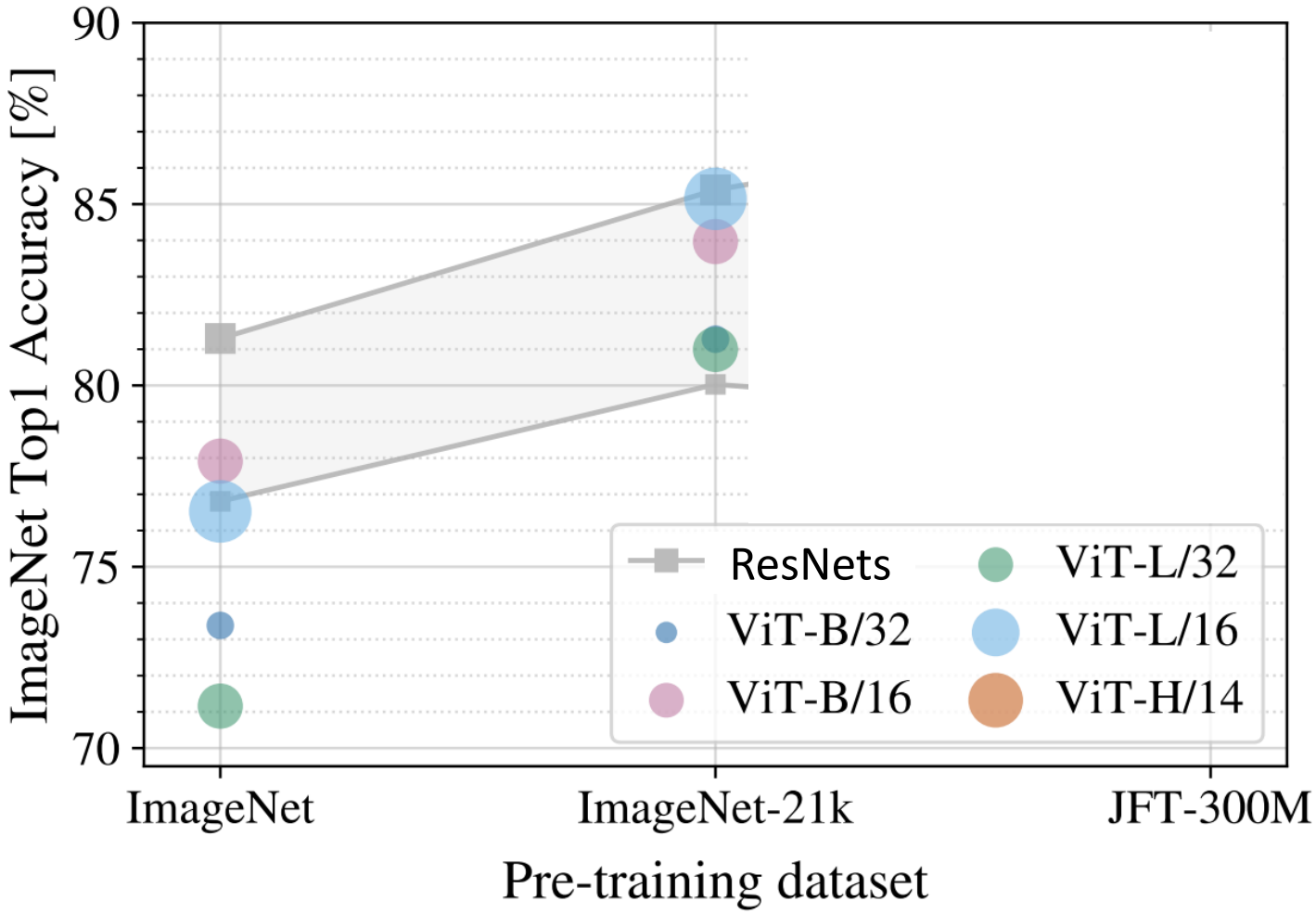
Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Vision Transformer (ViT) vs. ResNets

ImageNet-21k has 14M images with 21k categories

If you pretrain on ImageNet-21k and fine-tune on ImageNet, ViT does better: big ViTs match big ResNets



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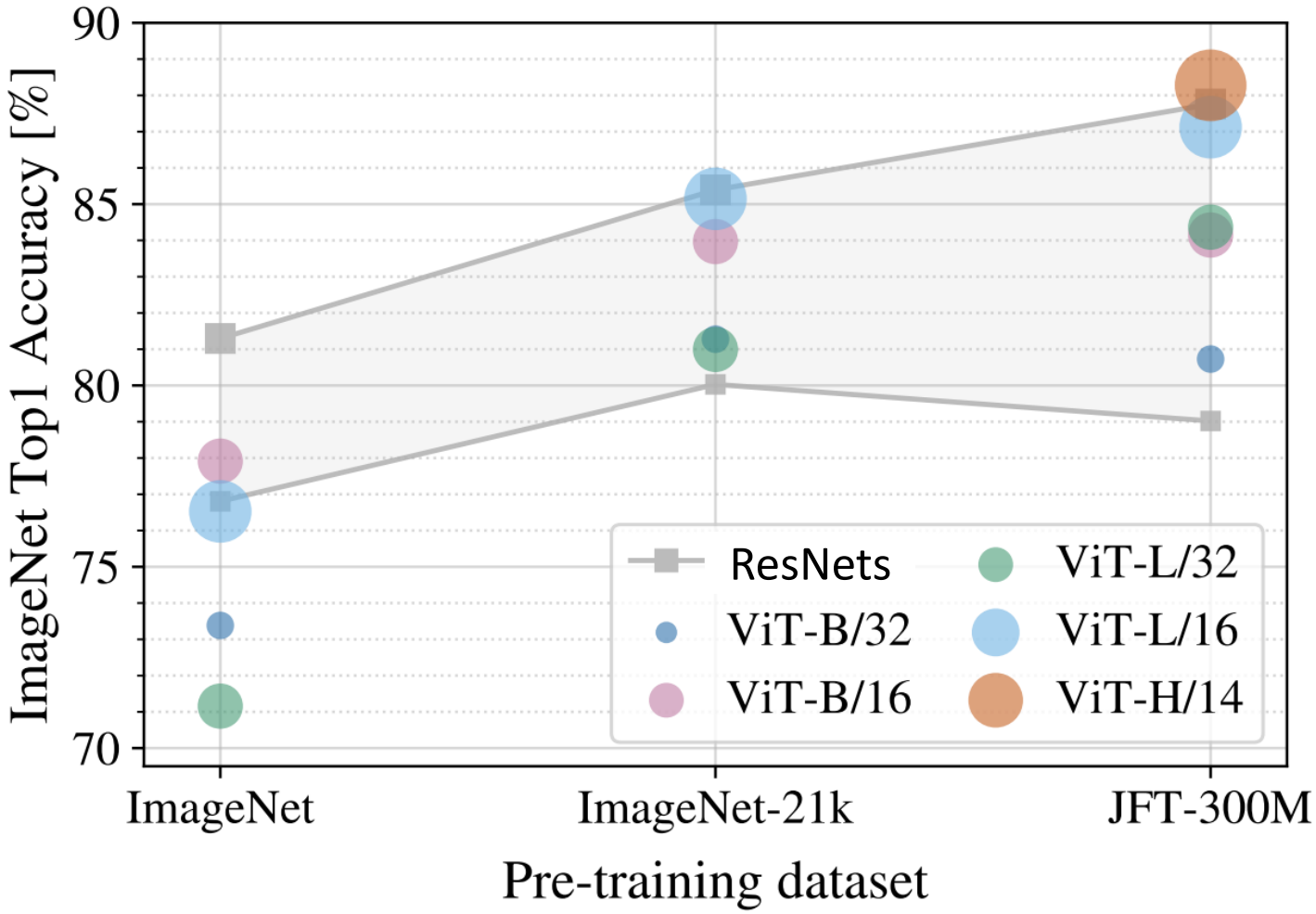
Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Vision Transformer (ViT) vs. ResNets

JFT-300M is an internal Google dataset with 300M labeled images

If you pretrain on JFT and finetune on ImageNet, large ViTs outperform large ResNets



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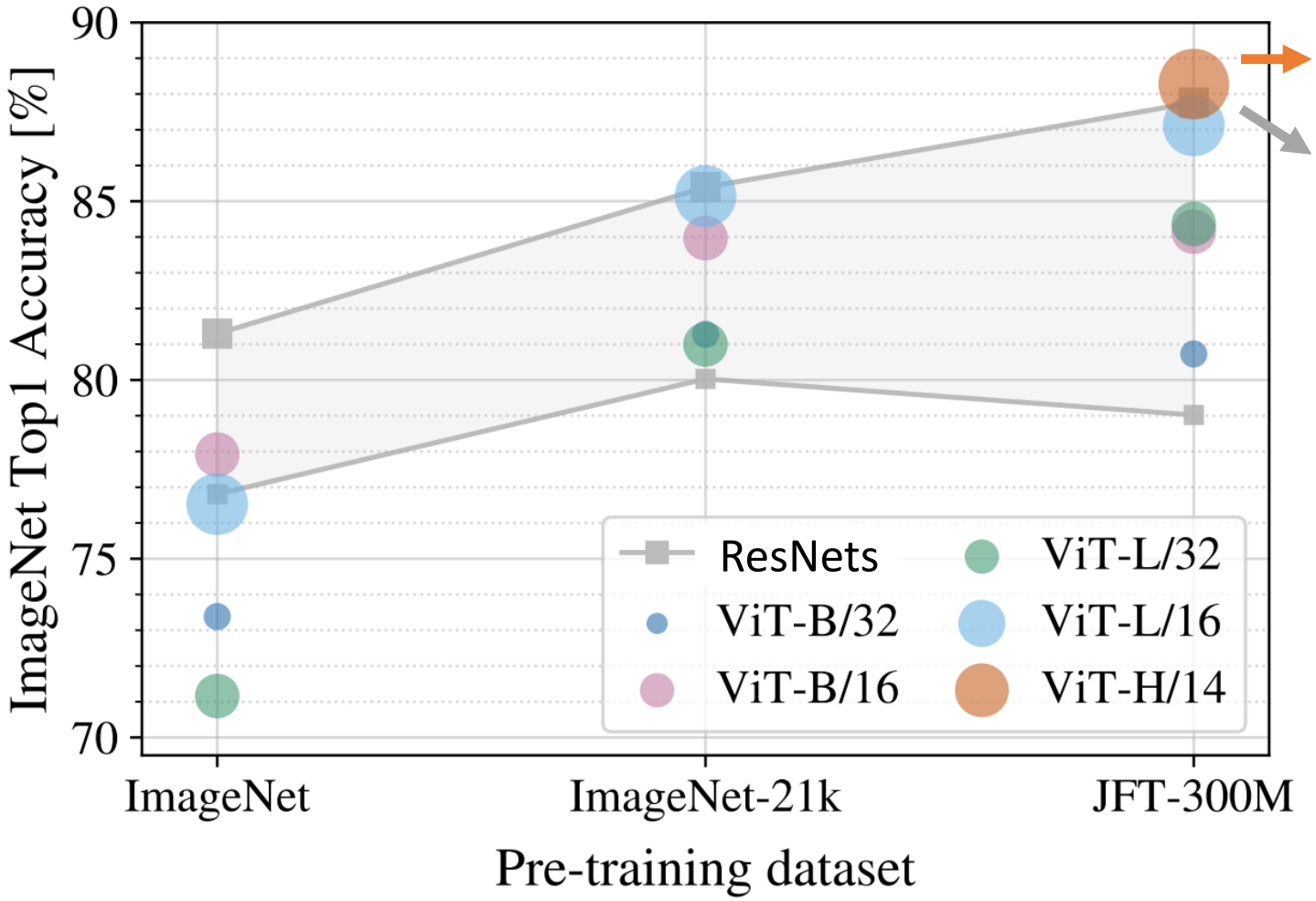


ViT: 2.5k TPU-v3 core days of training

ResNet: 9.9k TPU-v3 core days of training

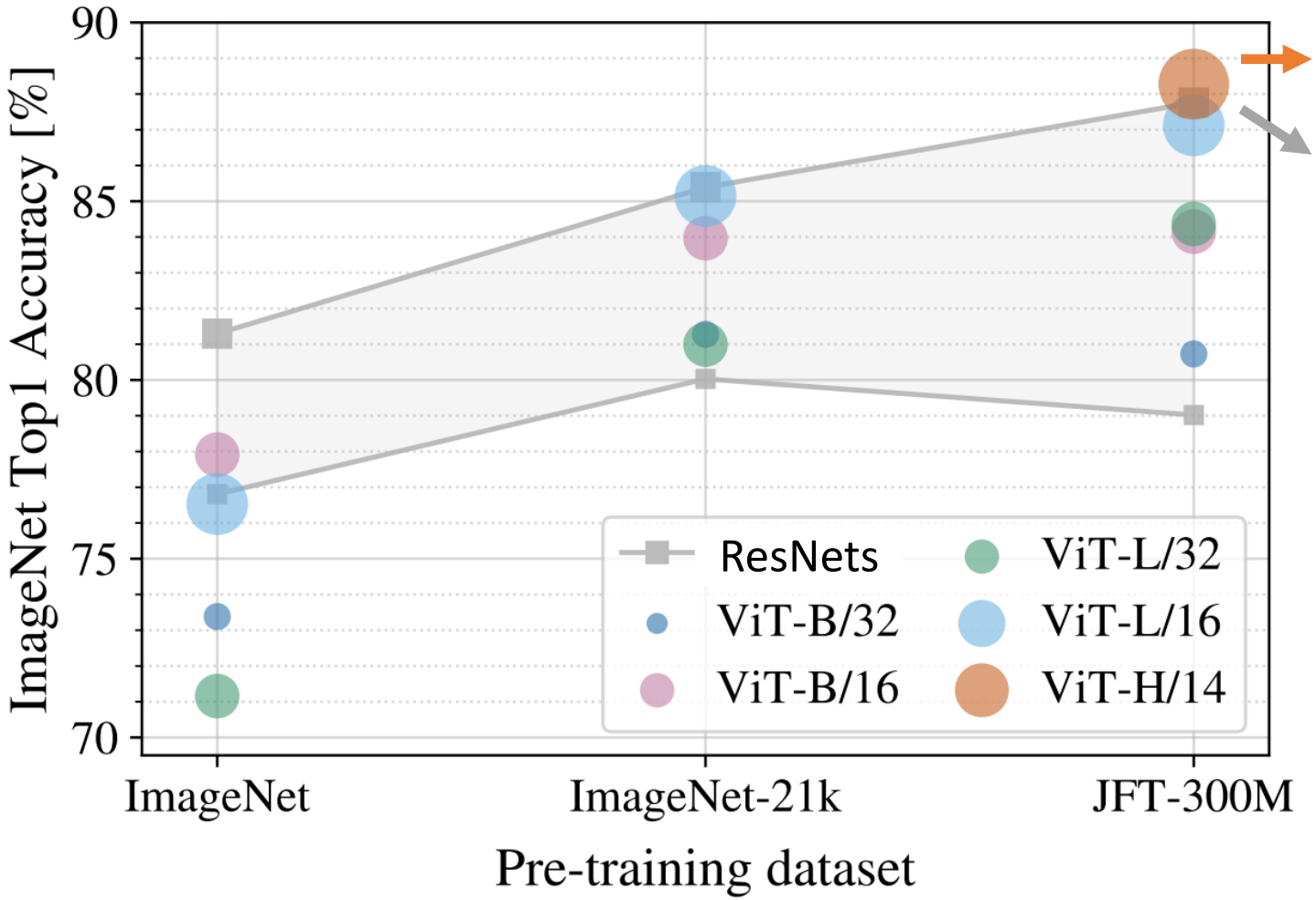
ViTs make more efficient use of GPU / TPU hardware (matrix multiply is more hardware-friendly than conv)

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Vision Transformer (ViT) vs. ResNets

Claim: ViT models have "less inductive bias" than ResNets, so need more pretraining data to learn good features

Not a very good explanation: "inductive bias" is not a well-defined concept we can measure!



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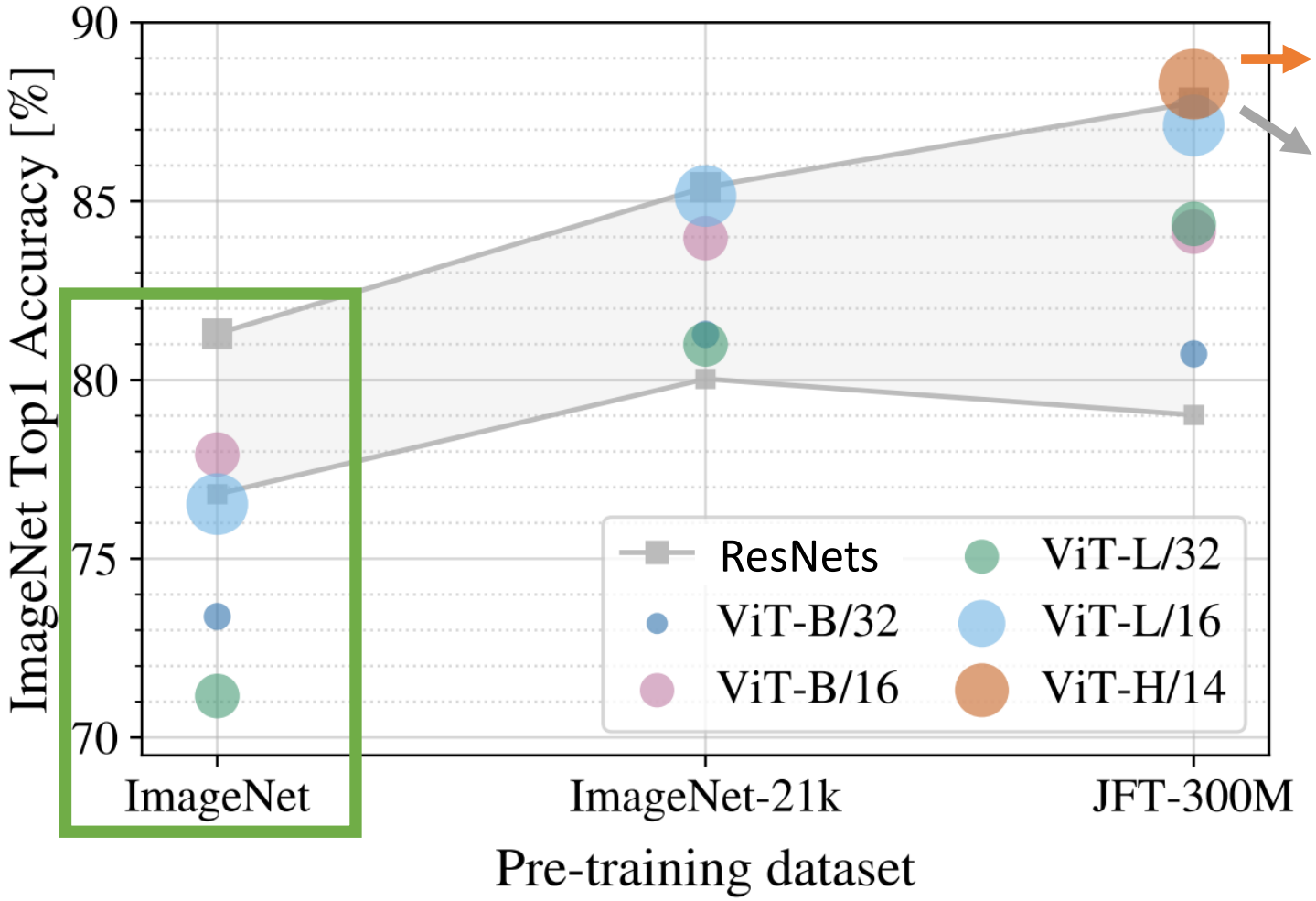
Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ICLR 2021

Vision Transformer (ViT) vs. ResNets

How can we improve the performance of ViT models on ImageNet?



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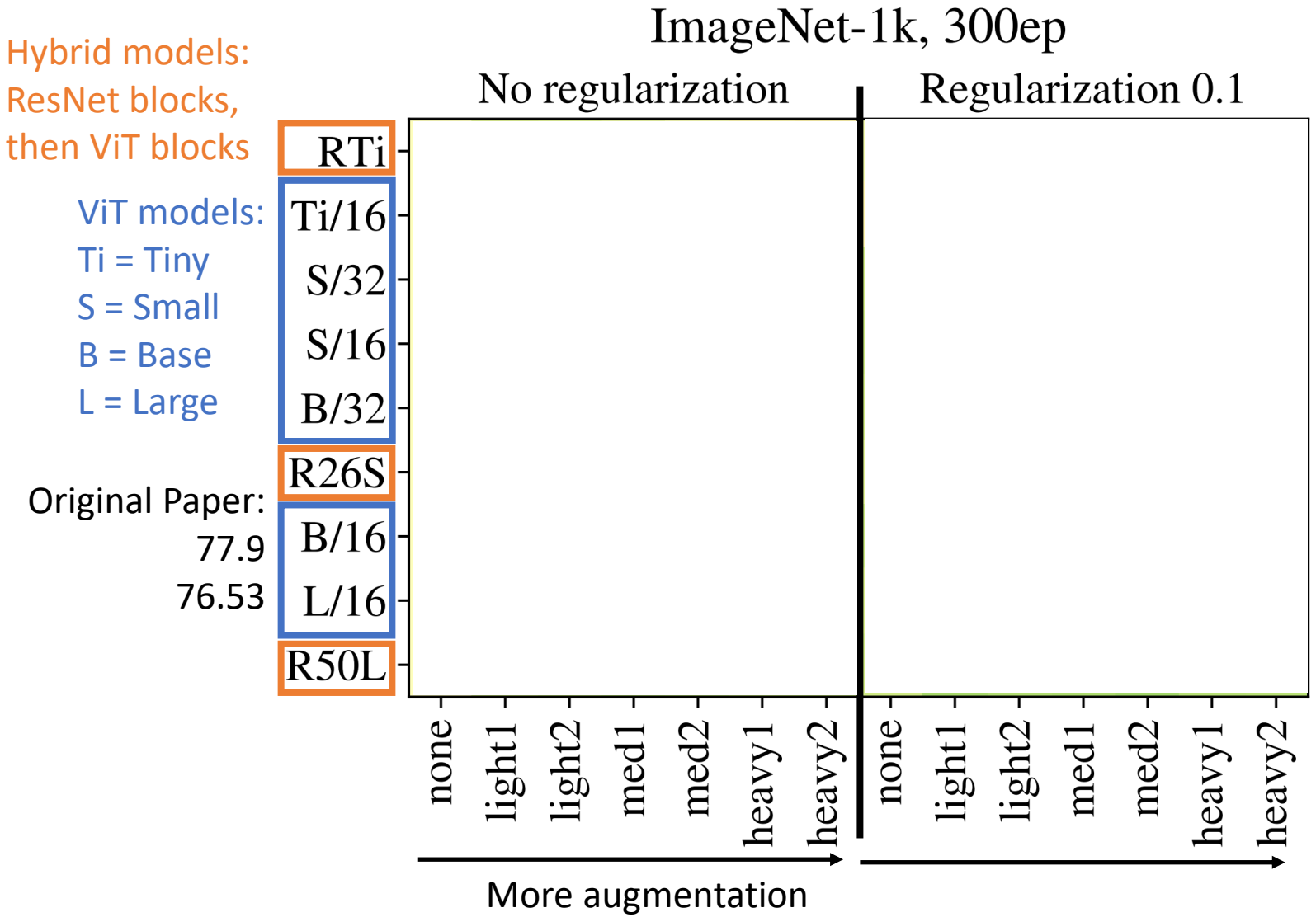
Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Improving ViT: Augmentation and Regularization

Regularization for ViT models:
- Weight Decay
- Stochastic Depth
- Dropout (in FFN layers of Transformer)

Data Augmentation for ViT models:
- MixUp
- RandAugment



Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Improving ViT: Augmentation and Regularization

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- Weight Decay
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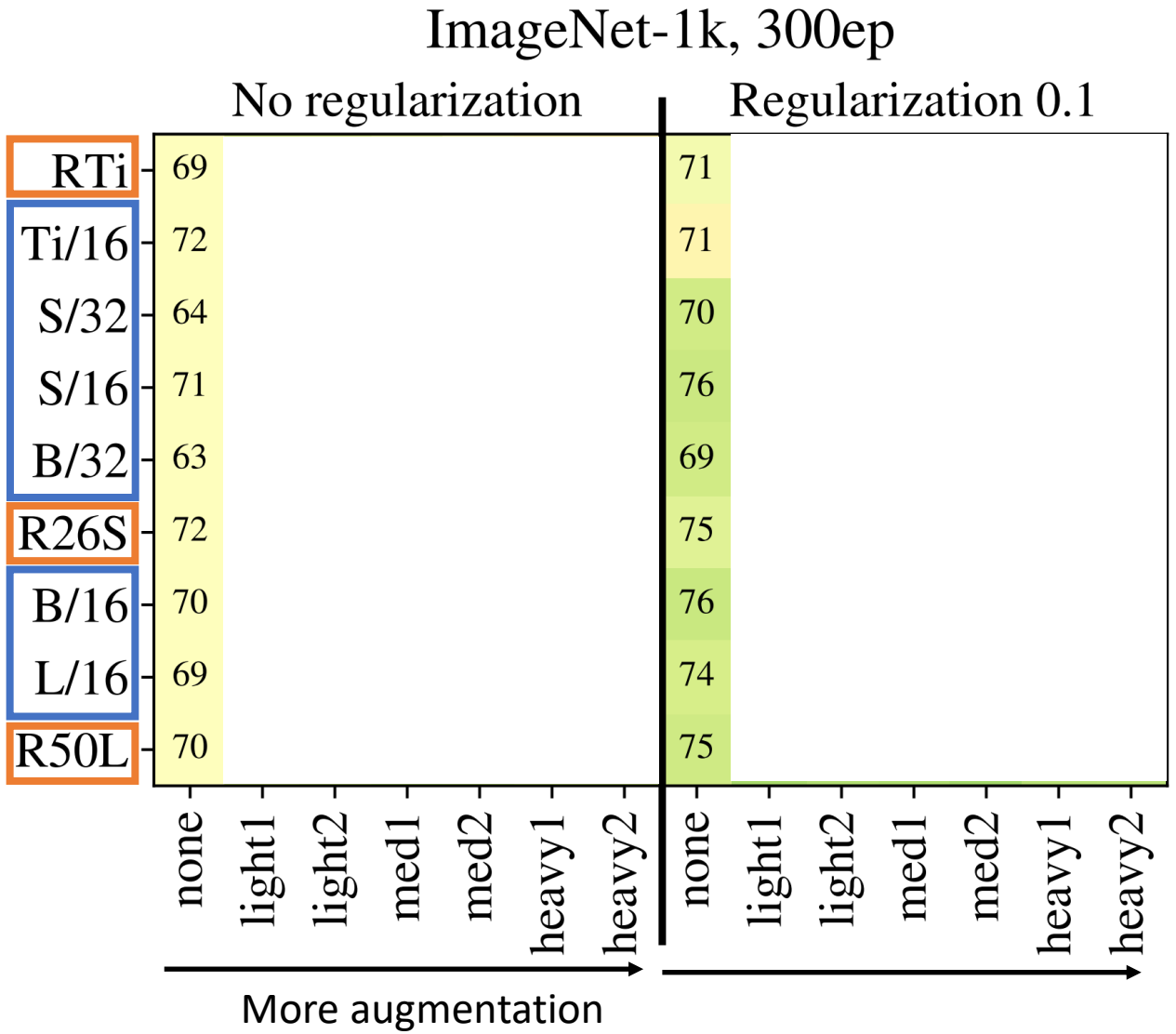
Data Augmentation for ViT models:
- MixUp
- RandAugment

Hybrid models: ResNet blocks, then ViT blocks

ViT models:
Ti = Tiny
S = Small
B = Base
L = Large

Original Paper:
77.9
76.53



Adding regularization is (almost) always helpful

Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Improving ViT: Augmentation and Regularization

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- Weight Decay
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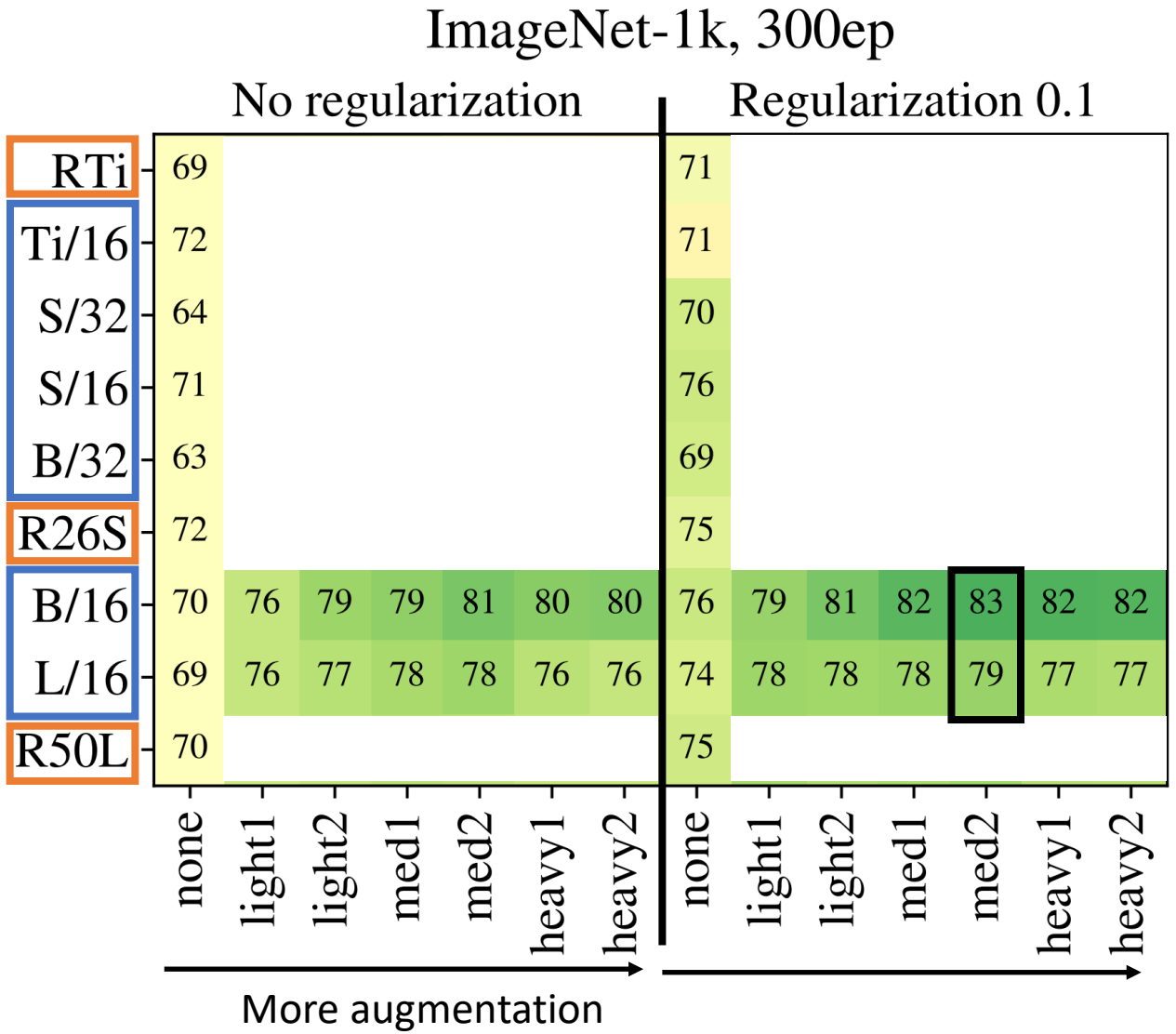
L = Large

Original Paper:
77.9
76.53

Regularization + Augmentation gives big improvements over original results



Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Improving ViT: Augmentation and Regularization

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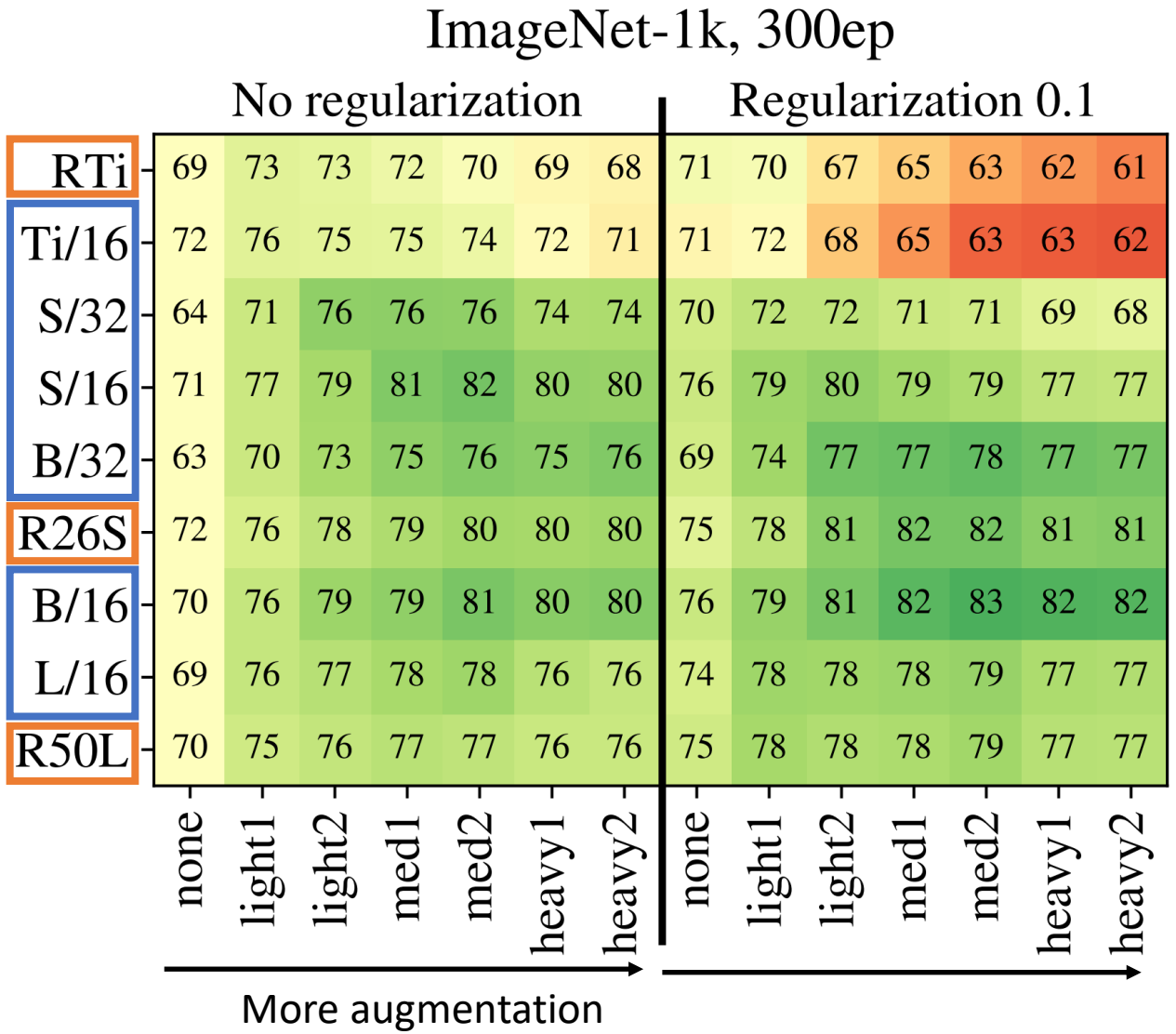
S = Small
B = Base
L = Large

Original Paper:
77.9
76.53

Lots of other patterns in full results

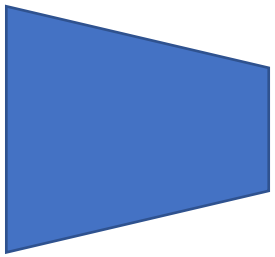


Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Improving ViT: Distillation

Often works better than training student from scratch (especially if teacher is bigger than student)

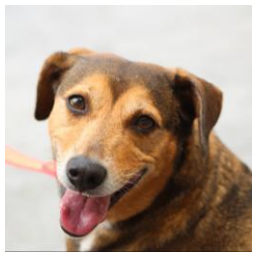
Step 1: Train a **teacher model** on images and ground-truth labels

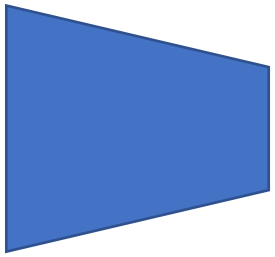


P(cat) = 0.9
P(dog) = 0.1

→ Cross Entropy Loss ← GT label: Cat

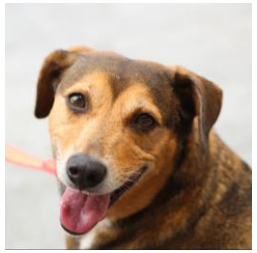
Step 2: Train a **student model** to match predictions from the **teacher** (sometimes also to match GT labels)

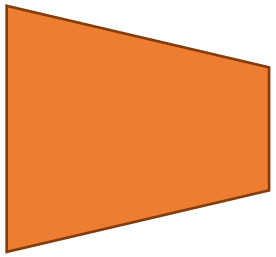




P(cat) = 0.1
P(dog) = 0.9

→ KL Divergence Loss





P(cat) = 0.2
P(dog) = 0.8

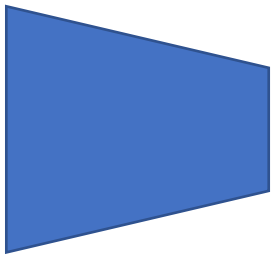
→ Cross Entropy Loss ← GT label: Dog

Hinton et al, "Distilling the knowledge in a neural network", NeurIPS Deep Learning and Representation Learning Workshop, 2015

Improving ViT: Distillation

Can also train student on **unlabeled** data! (Semi-supervised learning)

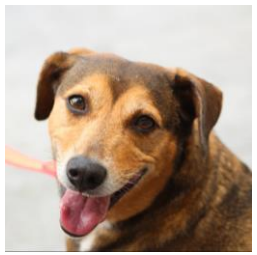
Step 1: Train a **teacher model** on images and ground-truth labels

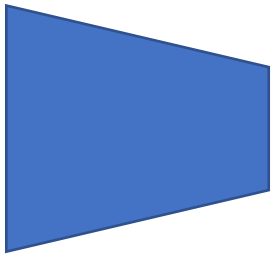


P(cat) = 0.9
P(dog) = 0.1

→ Cross Entropy Loss ← GT label: Cat

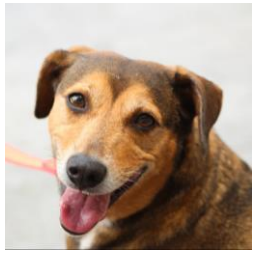
Step 2: Train a **student model** to match predictions from the **teacher** (sometimes also to match GT labels)

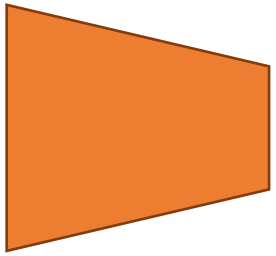




P(cat) = 0.1
P(dog) = 0.9

→ KL Divergence Loss





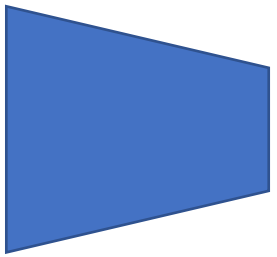
P(cat) = 0.2
P(dog) = 0.8

→ Cross Entropy Loss ← GT label: Dog

Hinton et al, "Distilling the knowledge in a neural network", NeurIPS Deep Learning and Representation Learning Workshop, 2015

Improving ViT: Distillation

Step 1: Train a **teacher CNN** on ImageNet



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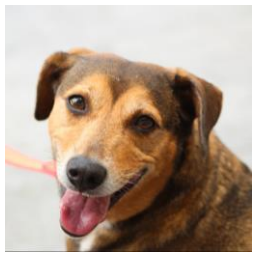
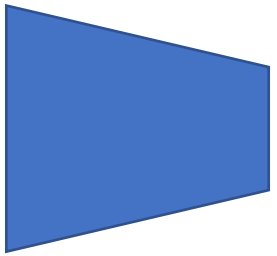
Step 2: Train a **student ViT** to match ImageNet predictions from the **teacher CNN** (and match GT labels)





P(cat) = 0.1
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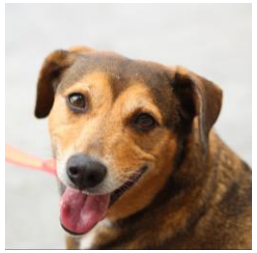
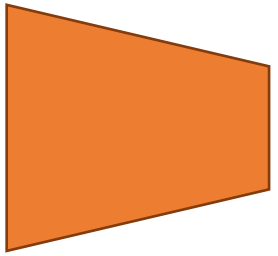
→ KL Divergence Loss





P(cat) = 0.2
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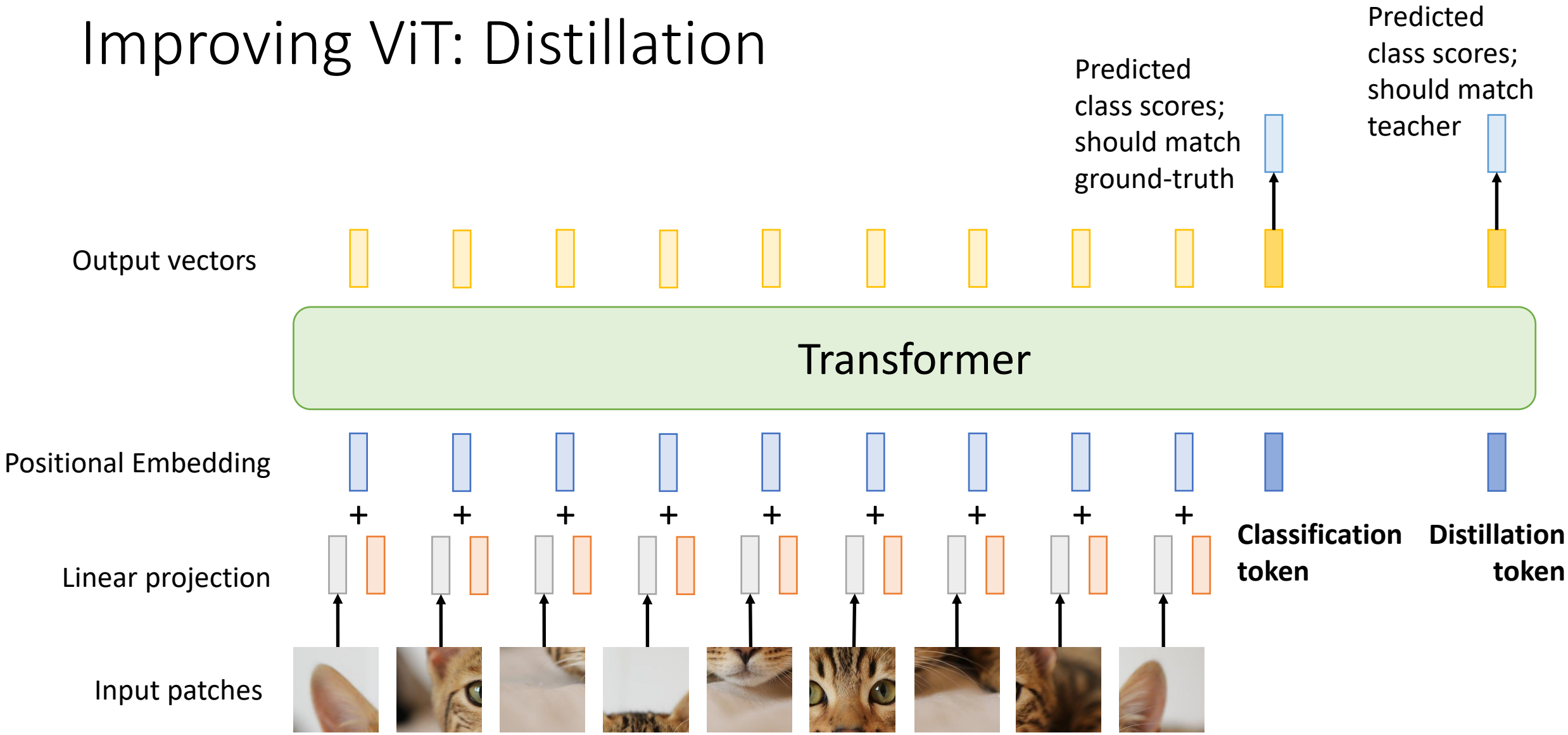
→ Cross Entropy Loss ← GT label: Dog

Touvrom et al, "Training data-efficient image transformers & distillation through attention", ICML 2021

Improving ViT: Distillation



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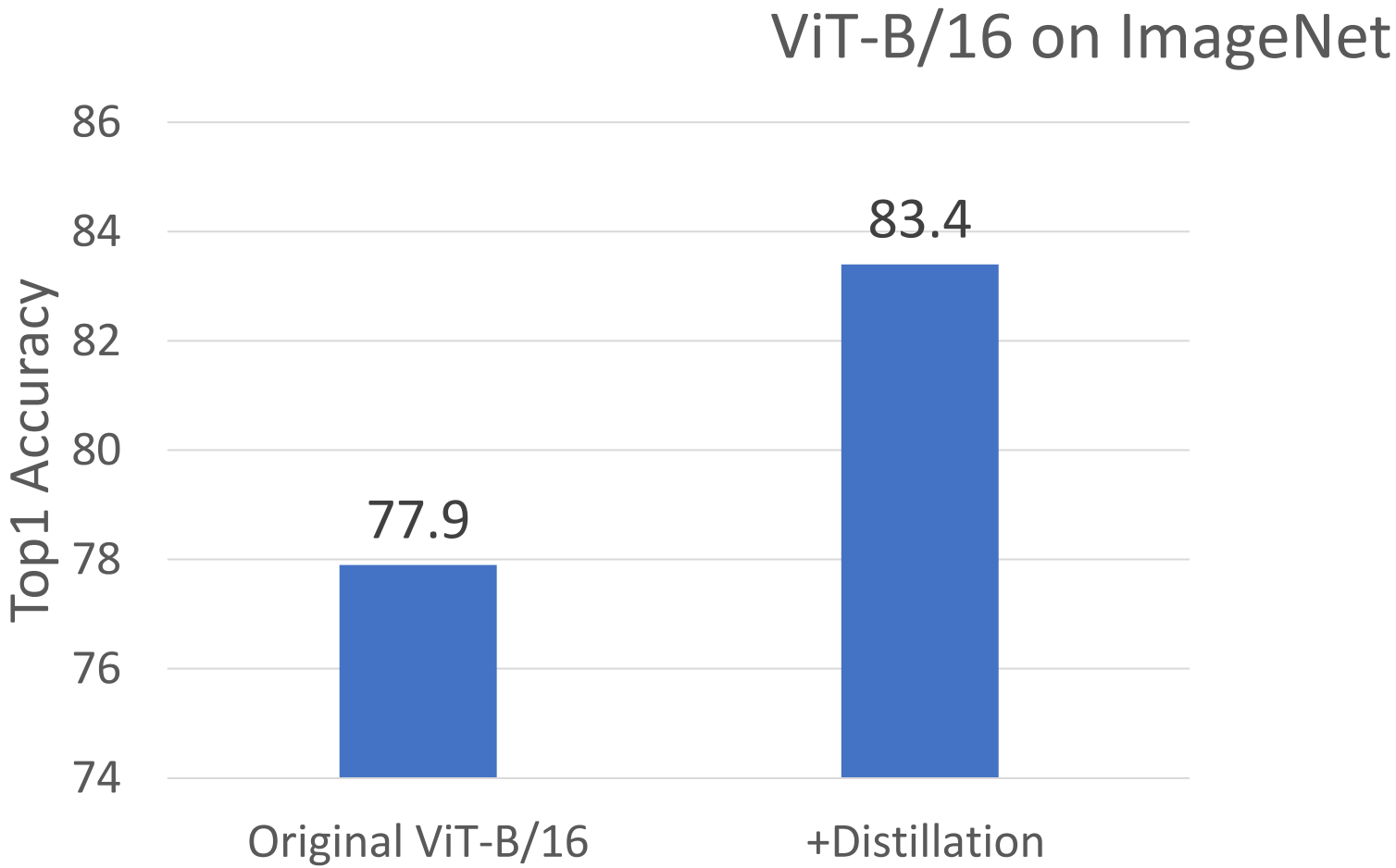
Improving ViT: Distillation



Touvrom et al, “Training data-efficient image transformers & distillation through attention”, ICML 2021

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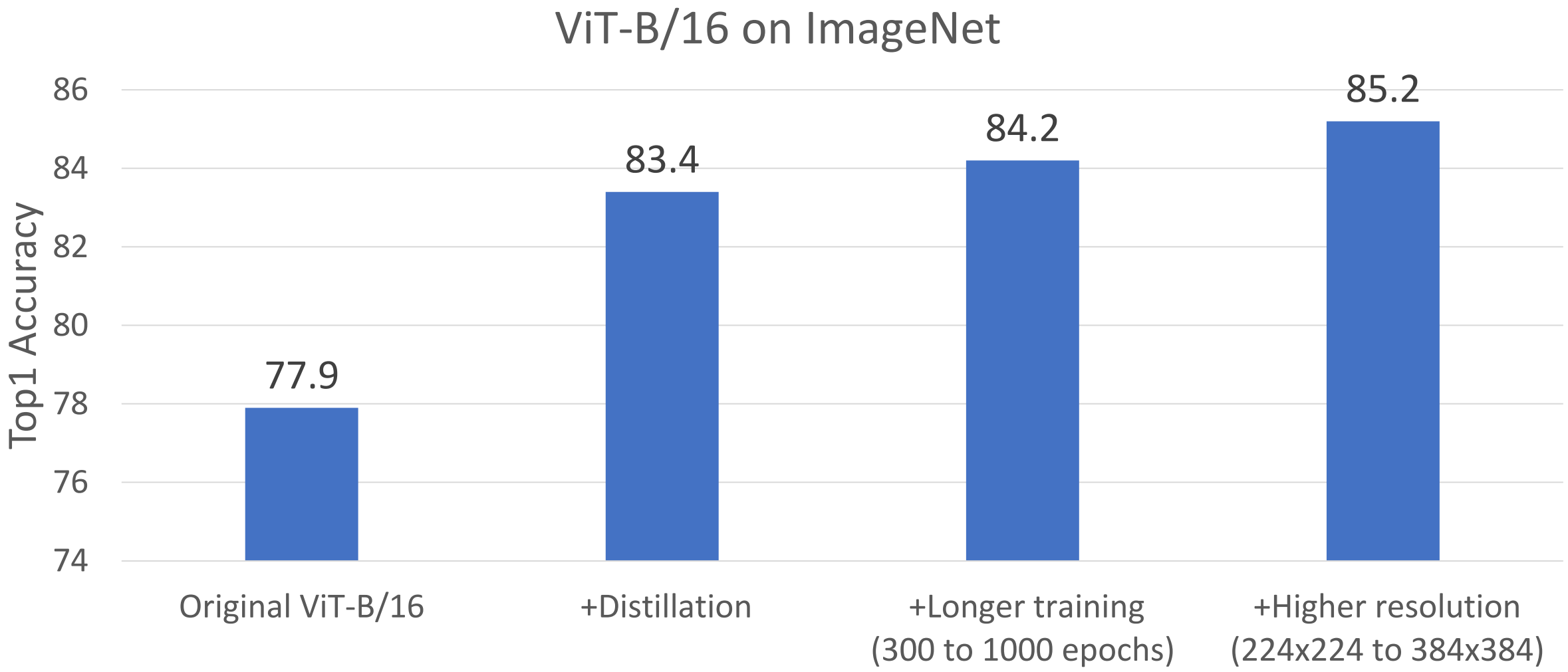
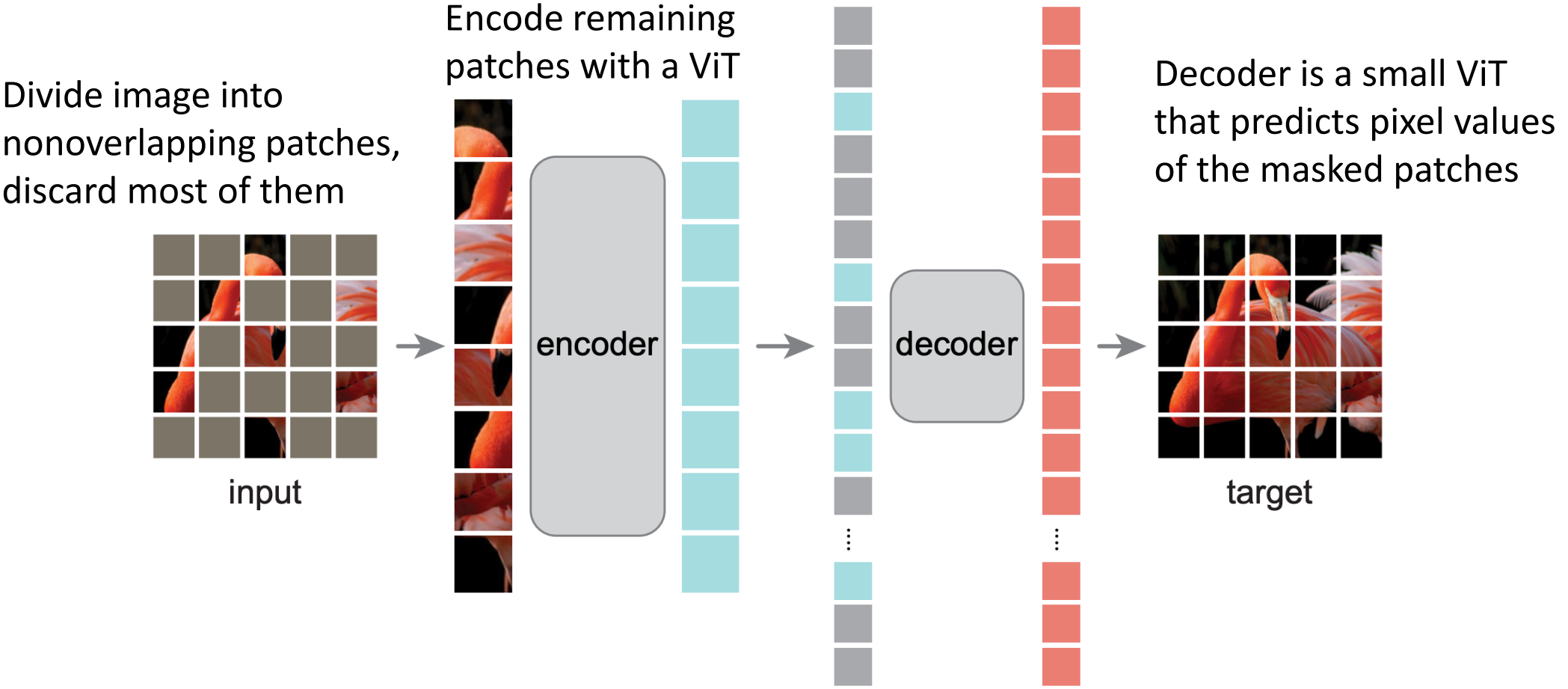


Touvrom et al, “Training data-efficient image transformers & distillation through attention”, ICML 2021

Improving ViT: Masked Autoencoders (MAE)

Self-Supervised Learning by Denoising Autoencoder with Vision Transformer



He et al, “Masked Autoencoders are Scalable Vision Learners”, CVPR 2022

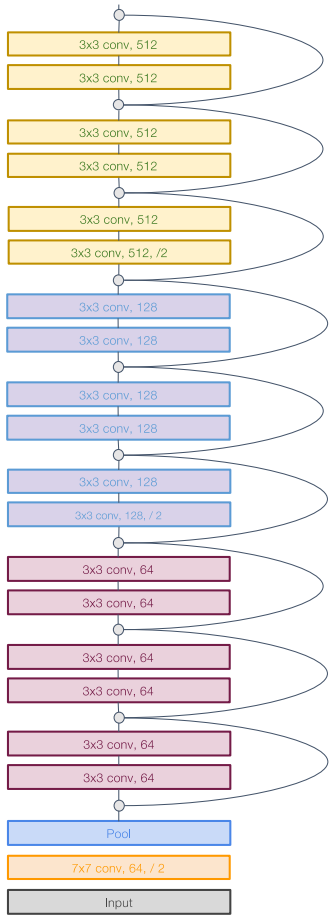
ViT vs. CNN

Stage 3:
256 x 14 x 14

Stage 2:
128 x 28 x 28

Stage 1:
64 x 56 x 56

Input:
3 x 224 x 224

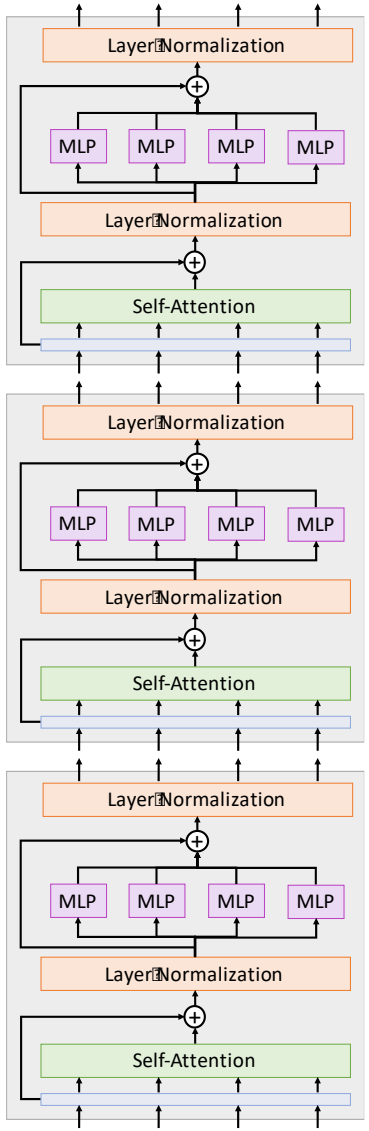


In most CNNs (including ResNets), **decrease** resolution and **increase** channels as you go deeper in the network (Hierarchical architecture)

Useful since objects in images can occur at various scales

In a ViT, all blocks have same resolution and number of channels (Isotropic architecture)

Can we build a **hierarchical** ViT model?



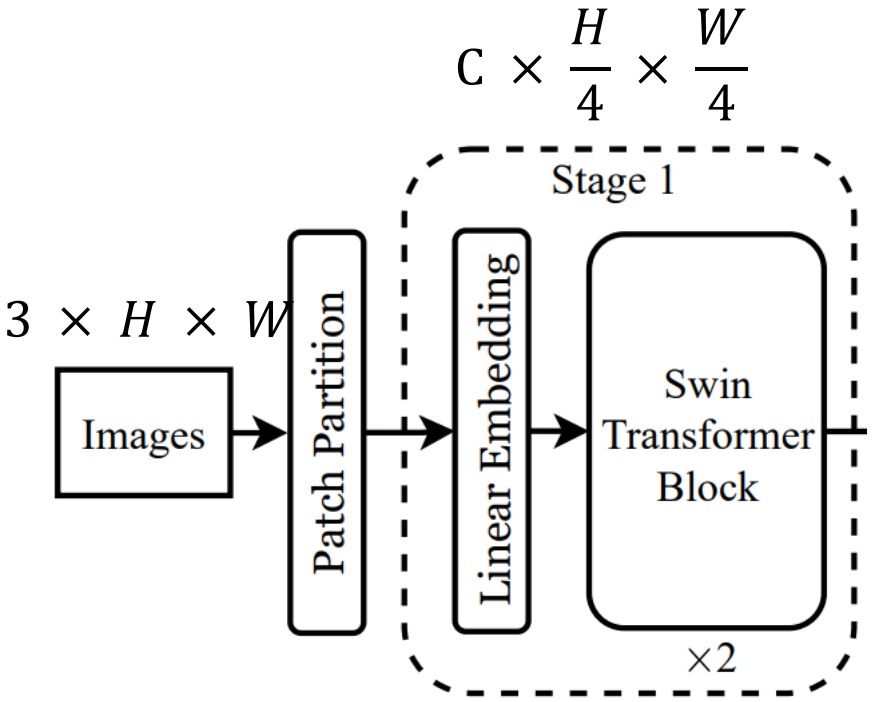
3rd block:
768 x 14 x 14

2nd block:
768 x 14 x 14

1st block:
768 x 14 x 14

Input:
3 x 224 x 224

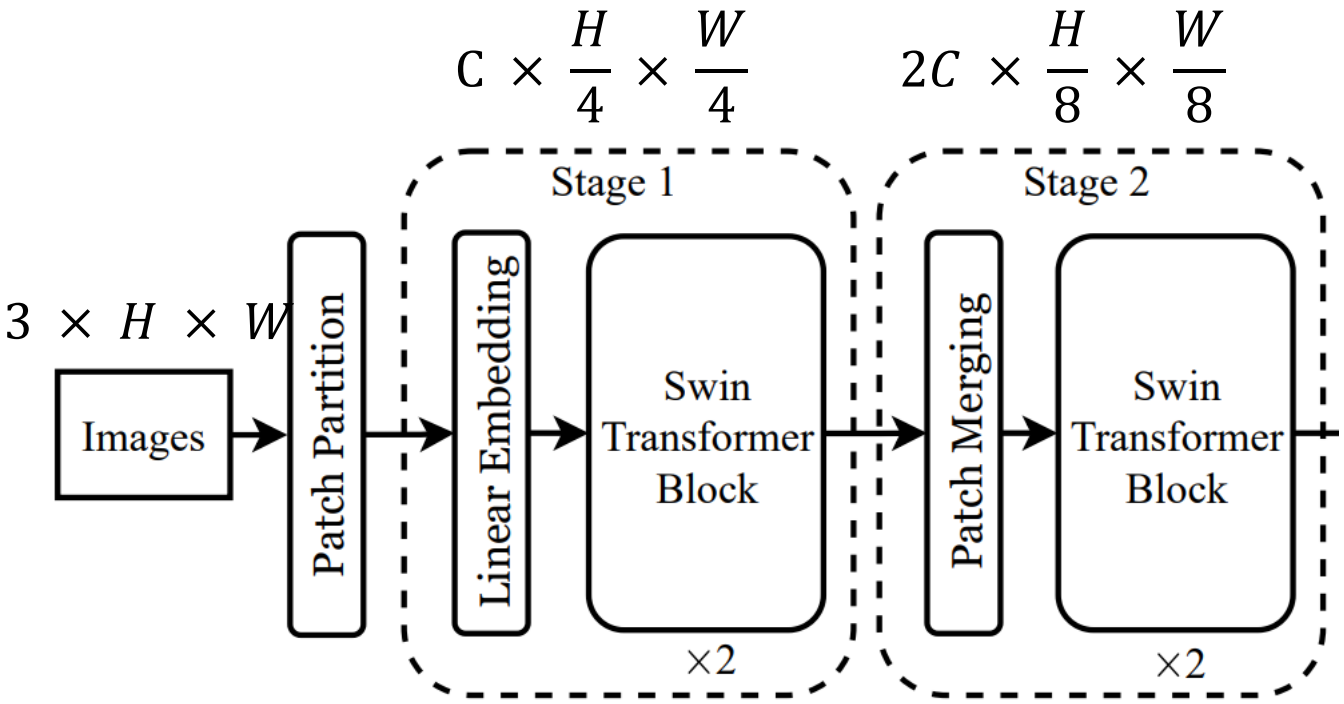
Hierarchical ViT: Swin Transformer

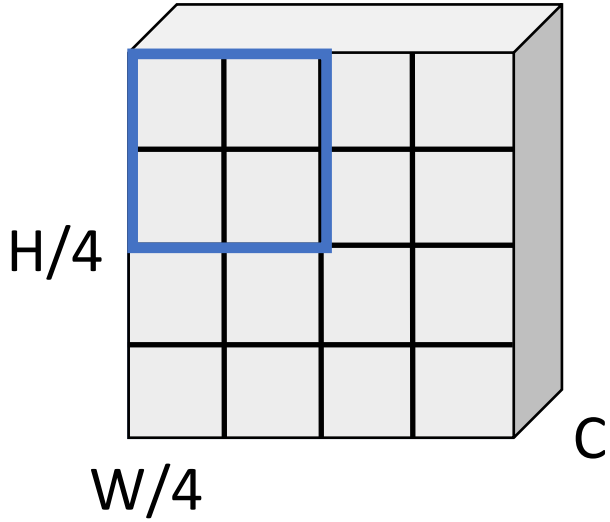


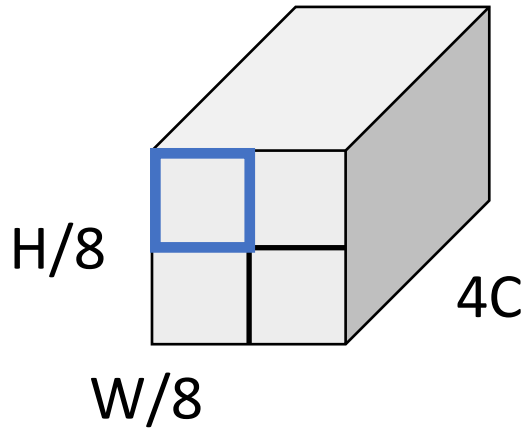
Divide image into 4x4 patches and project to C dimensions

Liu et al, “Swin Transformer: Hierarchical Vision Transformer using Shifted Windows”, CVPR 2021

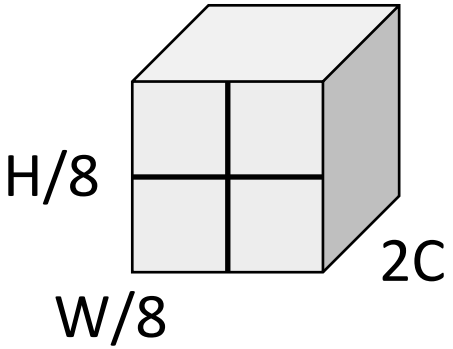
Hierarchical ViT: Swin Transformer







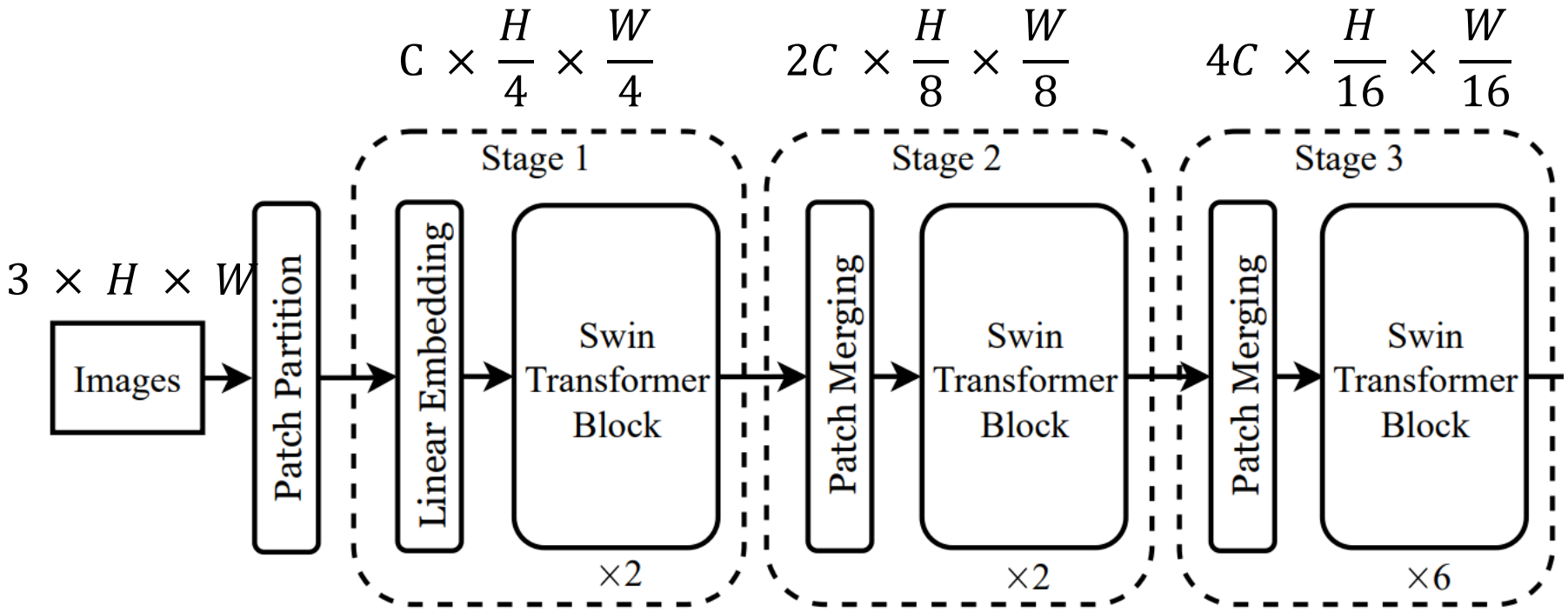
Concatenate groups of 2x2 features



Linear projection from 4C to 2C channels (1x1 conv)

Liu et al, “Swin Transformer: Hierarchical Vision Transformer using Shifted Windows”, CVPR 2021

Hierarchical ViT: Swin Transformer



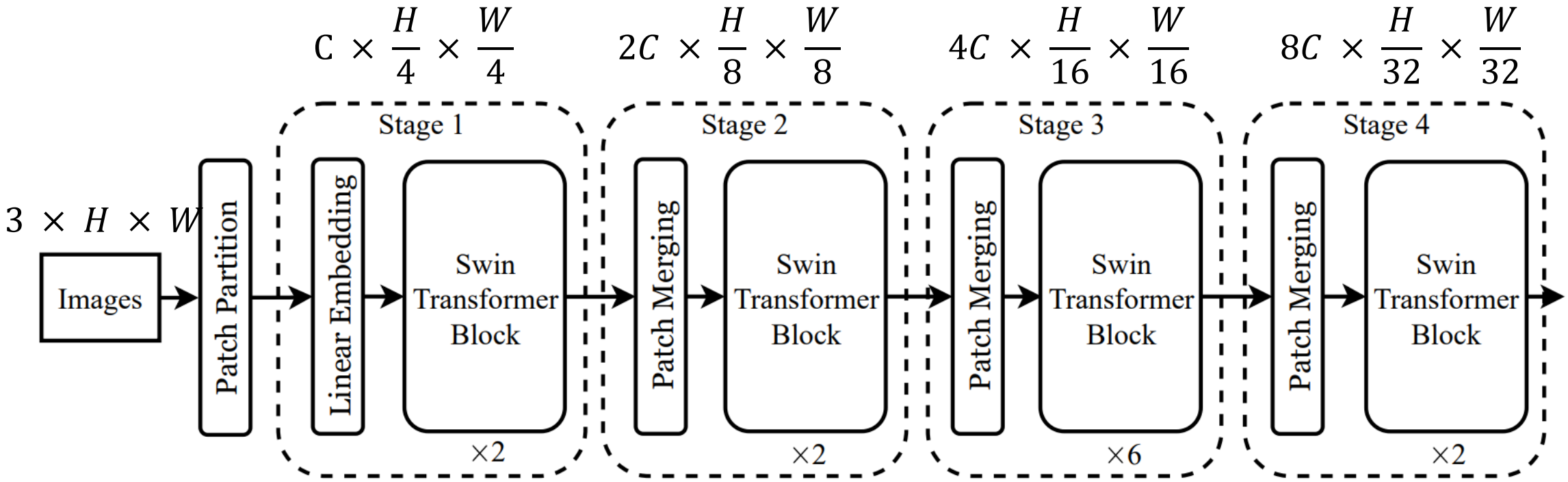
Divide image into 4x4 patches and project to C dimensions

Merge 2x2 neighborhoods; now patches are (effectively) 8x8

Merge 2x2 neighborhoods; now patches are (effectively) 16x16

Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

Hierarchical ViT: Swin Transformer



Divide image into 4x4 patches and project to C dimensions

Merge 2x2 neighborhoods; now patches are (effectively) 8x8

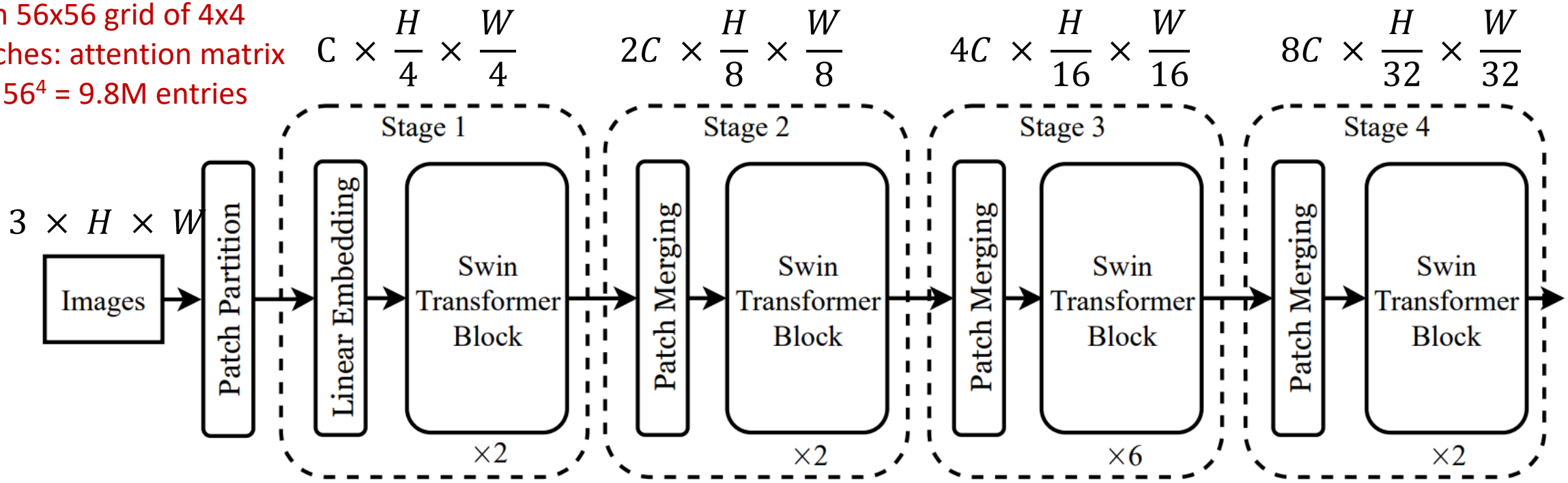
Merge 2x2 neighborhoods; now patches are (effectively) 16x16

Merge 2x2 neighborhoods; now patches are (effectively) 32x32

Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

Hierarchical ViT: Swin Transformer

Problem: 224x224 image with 56x56 grid of 4x4 patches: attention matrix has 56^4 = 9.8M entries



Solution: don't use full attention, instead use attention over patches

Divide image into 4x4 patches and project to C dimensions

Merge 2x2 neighborhoods; now patches are (effectively) 8x8

Merge 2x2 neighborhoods; now patches are (effectively) 16x16

Merge 2x2 neighborhoods; now patches are (effectively) 32x32

Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

Swin Transformer: Window Attention

With H x W grid of **tokens**, each attention matrix is H^2W^2 – **quadratic** in image size

Rather than allowing each **token** to attend to all other tokens, instead divide into **windows** of M x M tokens (here M=4); only compute attention within each window

Total size of all attention matrices is now:
$M^4(H/M)(W/M) = M^2HW$

Linear in image size for fixed M!
Swin uses M=7 throughout the network

Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

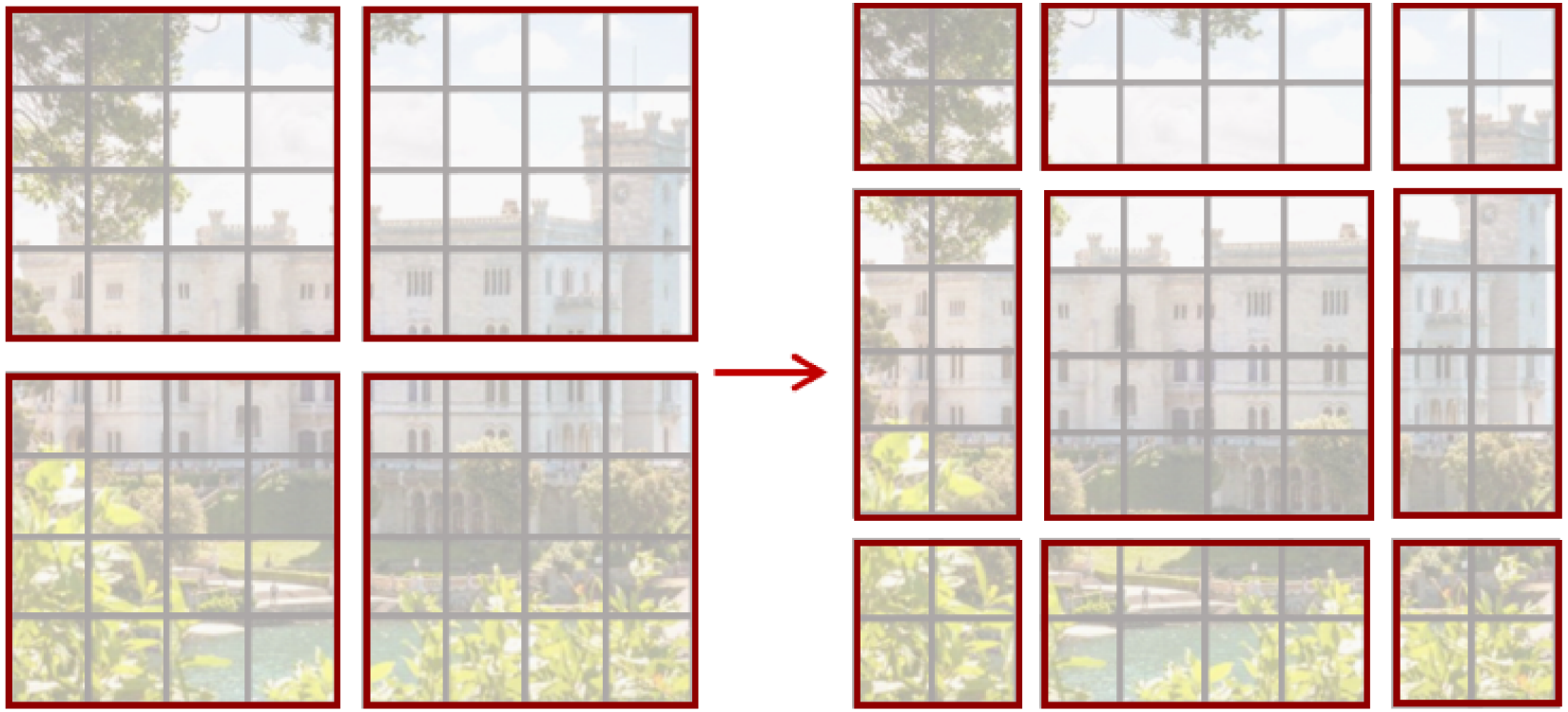
Swin Transformer: Window Attention

Problem: tokens only interact with other tokens within the same window; no communication across windows

Liu et al, “Swin Transformer: Hierarchical Vision Transformer using Shifted Windows”, CVPR 2021

Swin Transformer: Shifted Window Attention

Solution: Alternate between normal windows and shifted windows in successive Transformer blocks



Block L: Normal windows

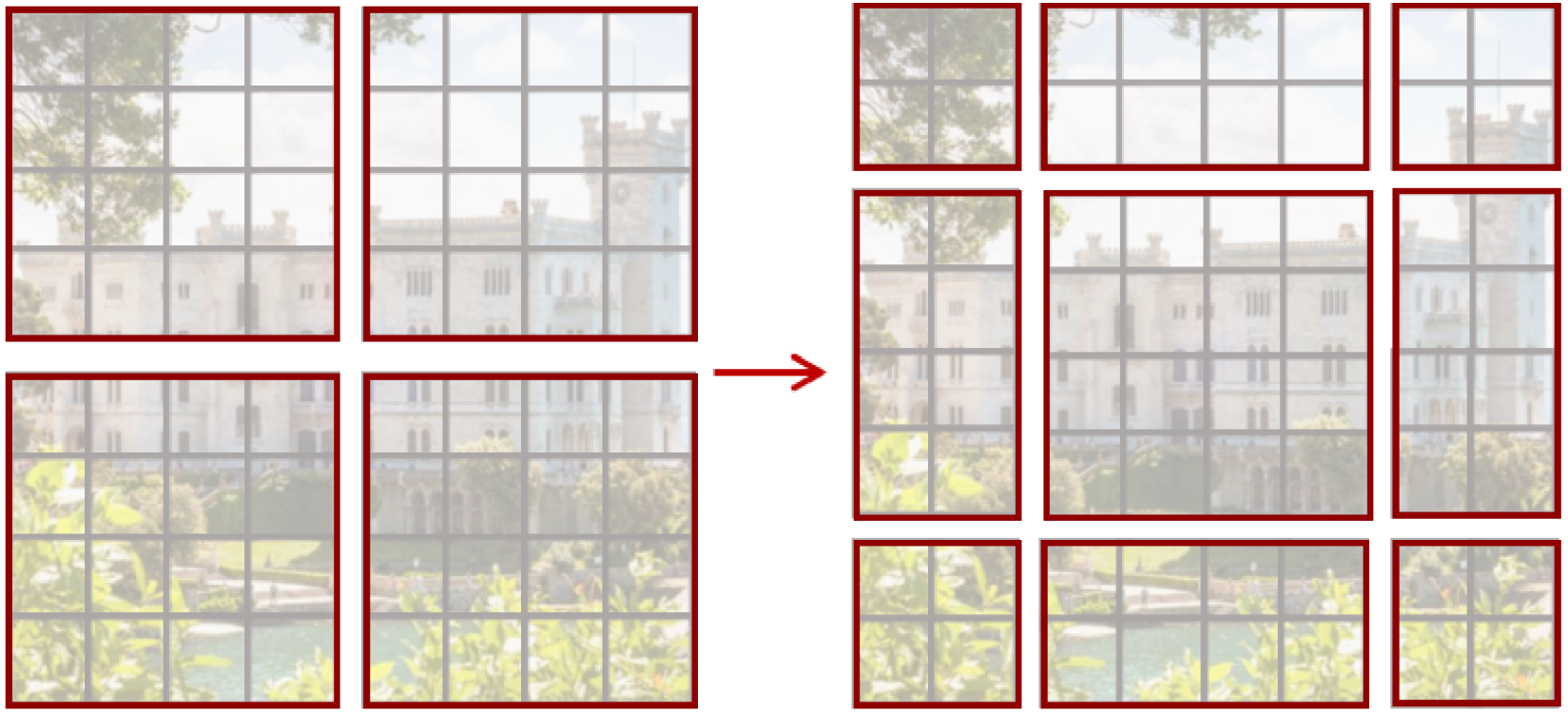
Block L+1: Shifted Windows

Ugly detail: Non-square windows at edges and corners

Liu et al, “Swin Transformer: Hierarchical Vision Transformer using Shifted Windows”, CVPR 2021

Swin Transformer: Shifted Window Attention

Solution: Alternate between normal windows and shifted windows in successive Transformer blocks



Block L: Normal windows

Block L+1: Shifted Windows

Detail: Relative Positional Bias

ViT adds positional embedding to input tokens, encodes *absolute position* of each token in the image

Swin does not use positional embeddings, instead encodes *relative position* between patches when computing attention:

Standard Attention:

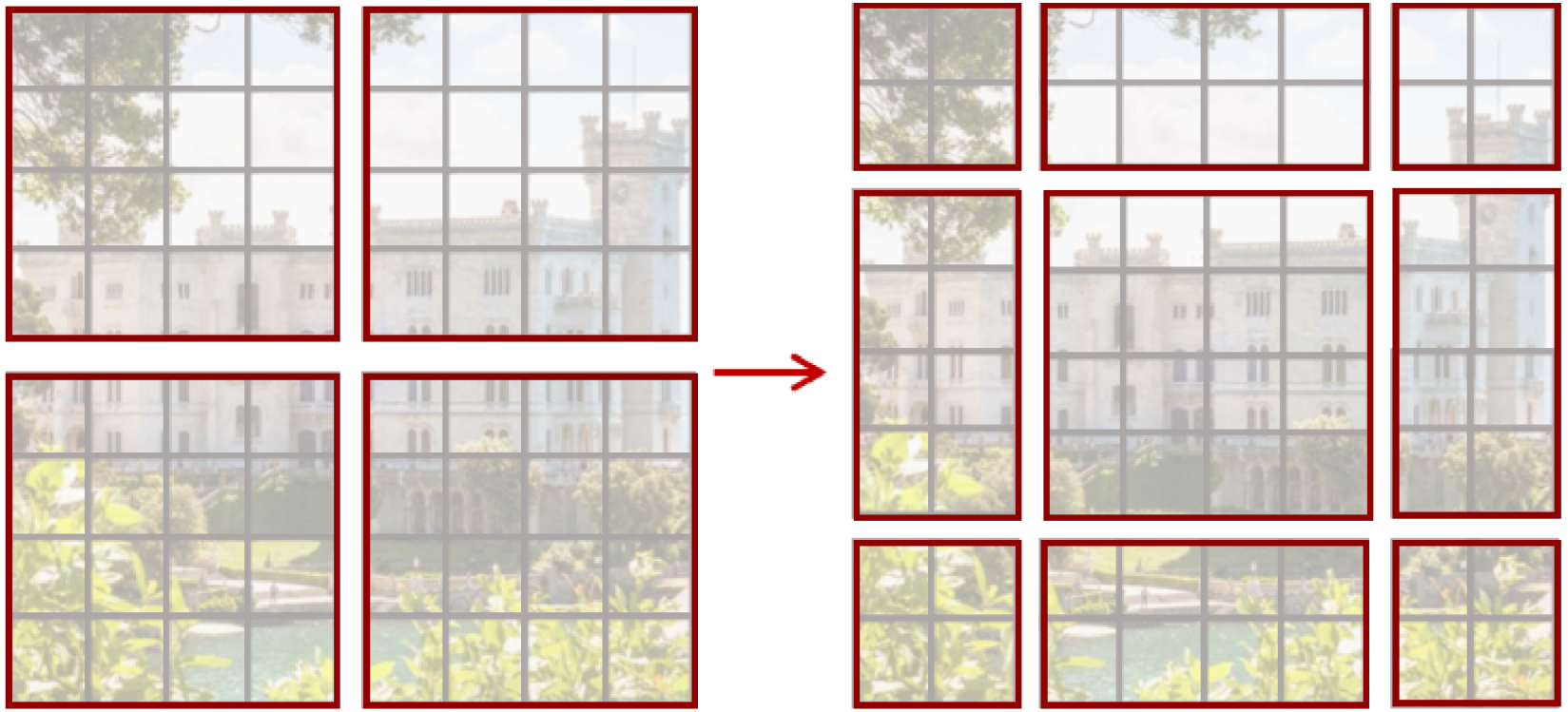
$$A = Softmax\left(\frac{QK^T}{\sqrt{D}}\right)V$$

$Q, K, V: M^2 \times D$ (Query, Key, Value)

Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

Swin Transformer: Shifted Window Attention

Solution: Alternate between normal windows and shifted windows in successive Transformer blocks



Block L: Normal windows

Block L+1: Shifted Windows

Detail: Relative Positional Bias

ViT adds positional embedding to input tokens, encodes *absolute position* of each token in the image

Swin does not use positional embeddings, instead encodes *relative position* between patches when computing attention:

Attention with relative bias:

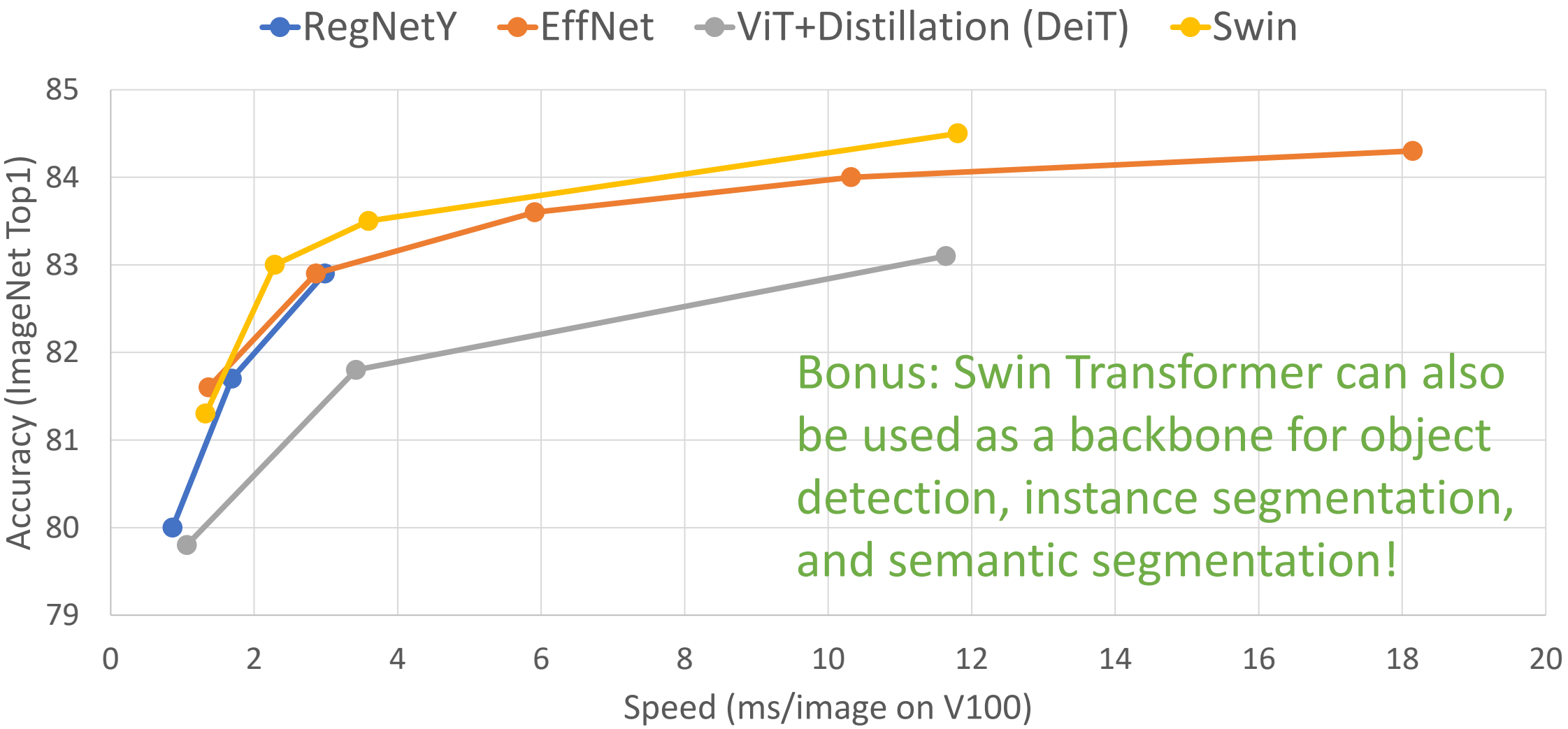
$$A = Softmax\left(\frac{QK^T}{\sqrt{D}} + B\right)V$$

$Q, K, V: M^2 \times D$ (Query, Key, Value)

$B: M^2 \times M^2$ (learned biases)

Liu et al, "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows", CVPR 2021

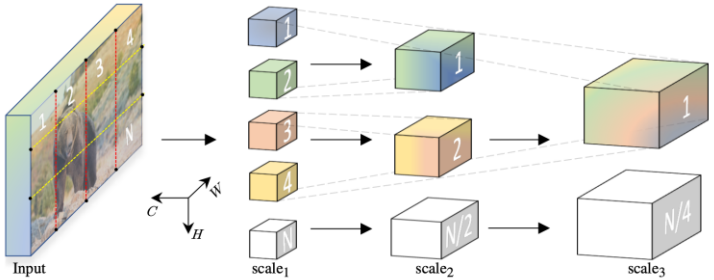
Swin Transformer: Speed vs. Accuracy



Liu et al, “Swin Transformer: Hierarchical Vision Transformer using Shifted Windows”, CVPR 2021

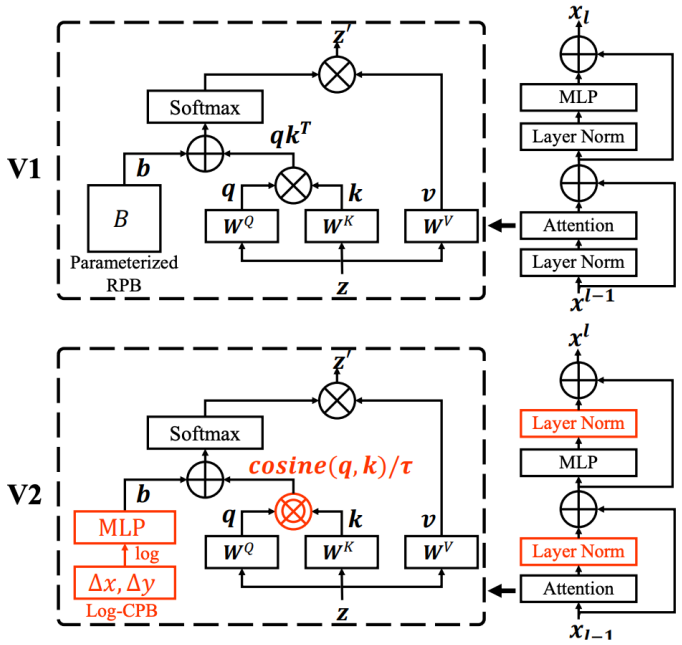
Other Hierarchical Vision Transformers

MViT



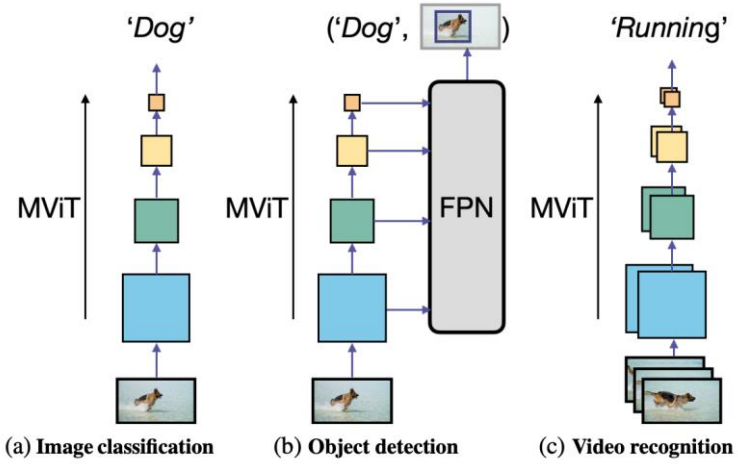
Fan et al, “Multiscale Vision Transformers”, ICCV 2021

Swin-V2



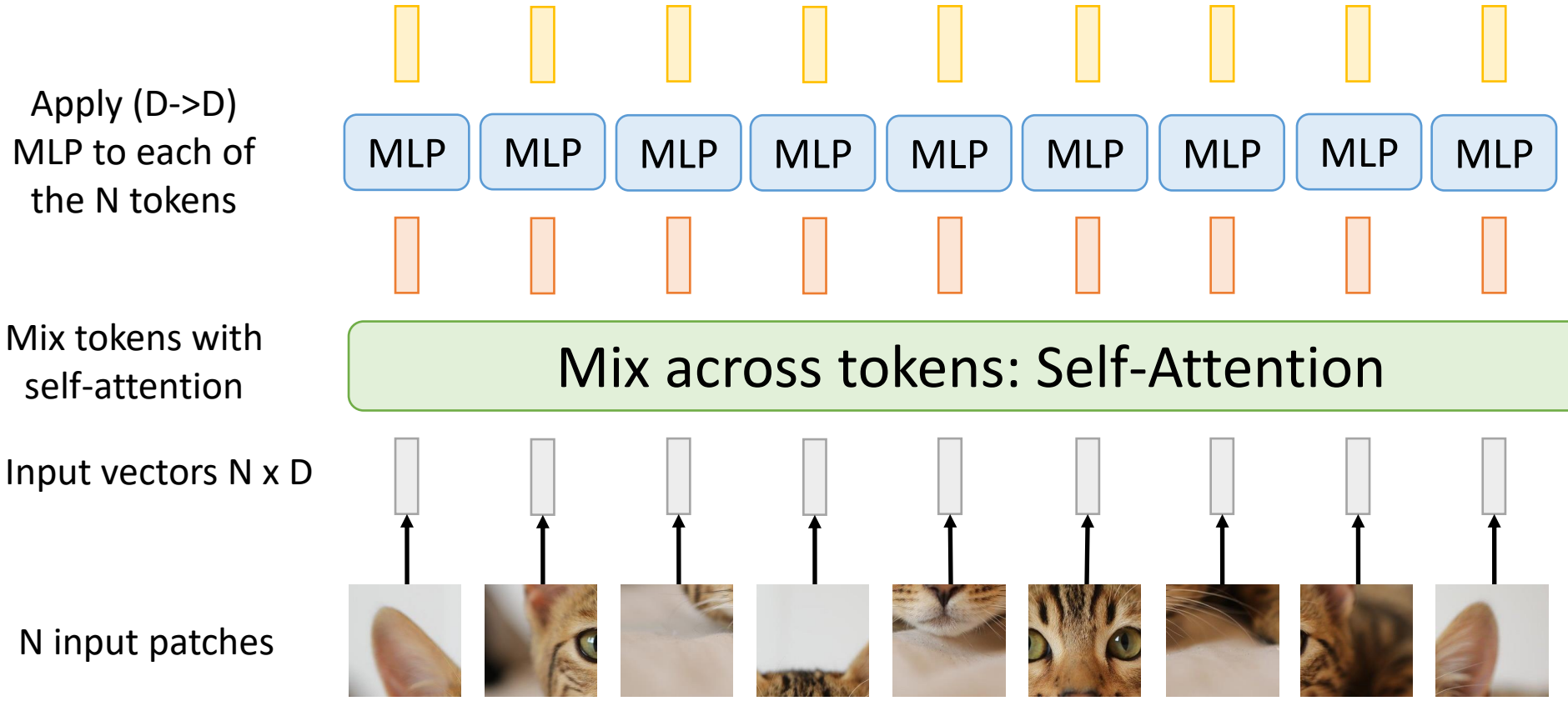
Liu et al, “Swin Transformer V2: Scaling up Capacity and Resolution”, CVPR 2022

Improved MViT



Li et al, “Improved Multiscale Vision Transformers for Classification and Detection”, arXiv 2021

Vision Transformer: Another Look



Question: Can we use something simpler than self-attention to mix across tokens?

Dosovitskiy et al, "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale", ICLR 2021

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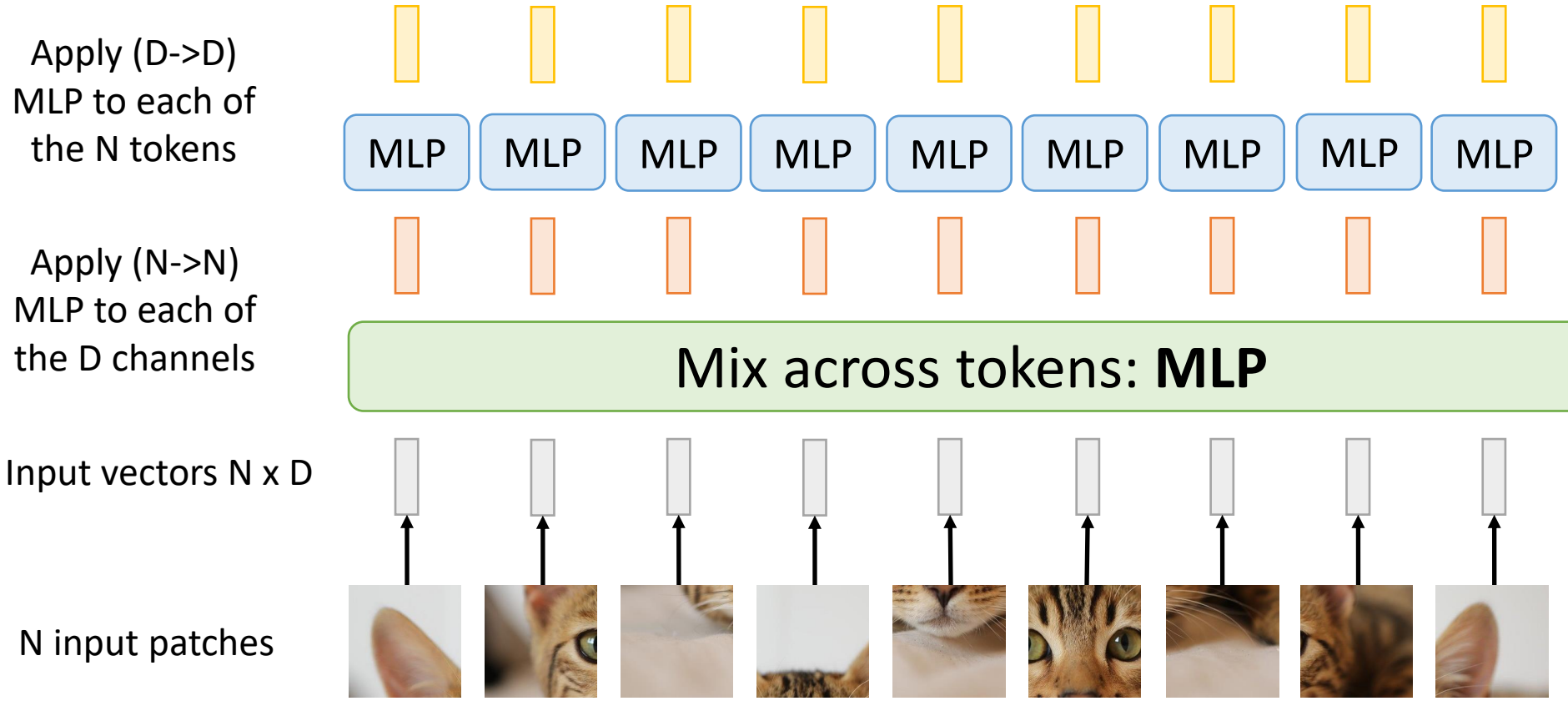
MLP-Mixer: An All-MLP Architecture



Question: Can we use something simpler than self-attention to mix across tokens?

Tolstikhin et al, "MLP-Mixer: An all-MLP architecture for vision", NeurIPS 2021

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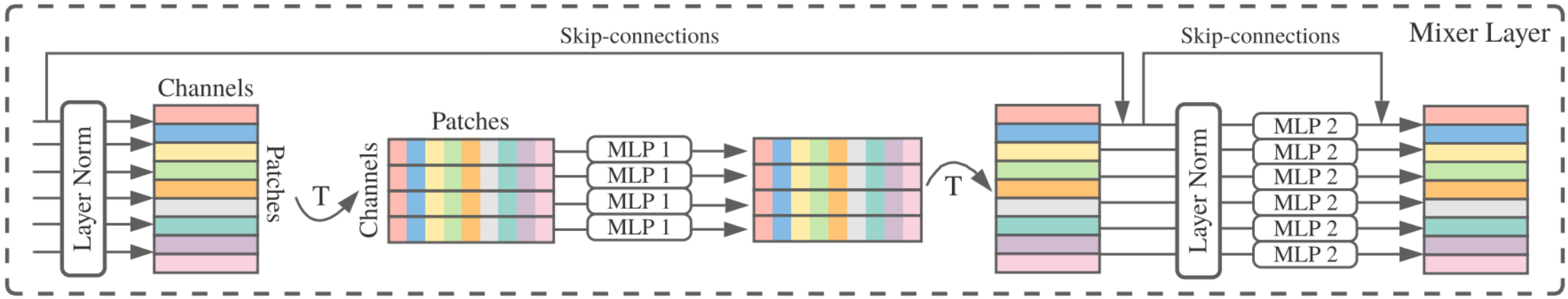
MLP-Mixer: An All-MLP Architecture



Input: N x C
N patches with
C channels each

MLP 1: C -> C,
apply to each of
the **N patches**

MLP 2: N -> N,
apply to each of
the **C channels**

Tolstikhin et al, “MLP-Mixer: An all-MLP architecture for vision”, NeurIPS 2021

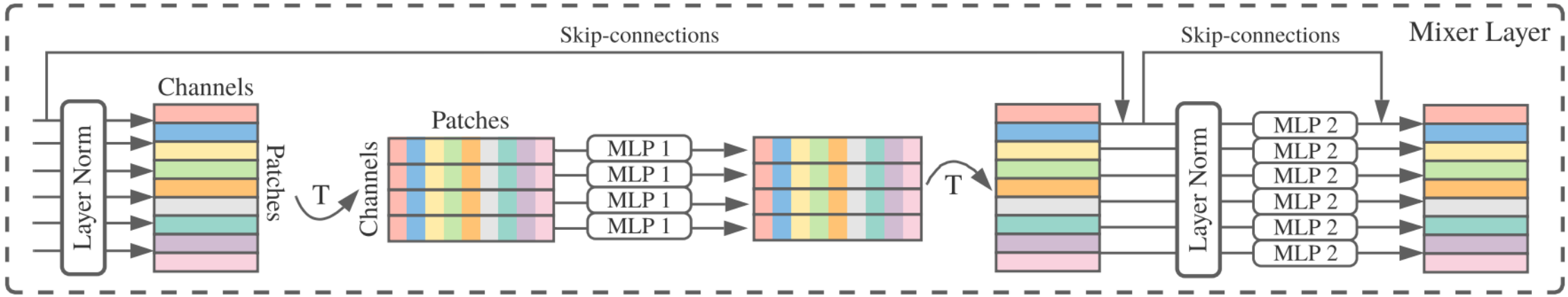
MLP-Mixer: An All-MLP Architecture

Cool idea; but initial ImageNet results not very compelling (but better with JFT pretraining)

MLP-Mixer is actually just a weird CNN???

Equivalent to
Conv(1x1, C->C, stride=1)

Equivalent to
Conv($N^{1/2}$ x $N^{1/2}$, C->C, groups=C)



Input: N x C
N patches with
C channels each

MLP 1: C -> C,
apply to each of
the **N patches**

MLP 2: N -> N,
apply to each of
the **C channels**

Tolstikhin et al, “MLP-Mixer: An all-MLP architecture for vision”, NeurIPS 2021

MLP-Mixer: Many Concurrent and Follow-ups

Touvron et al, “ResMLP: Feedforward Networks for Image Classification with Data-Efficient Training”, arXiv 2021, https://arxiv.org/abs/2105.03404

Tolstikhin et al, “MLP-Mixer: An all-MLP architecture for vision”, NeurIPS 2021, https://arxiv.org/abs/2105.01601

Liu et al, “Pay Attention to MLPs”, NeurIPS 2021, https://arxiv.org/abs/2105.08050

Yu et al, “S2-MLP: Spatial-Shift MLP Architecture for Vision”, WACV 2022, https://arxiv.org/abs/2106.07477

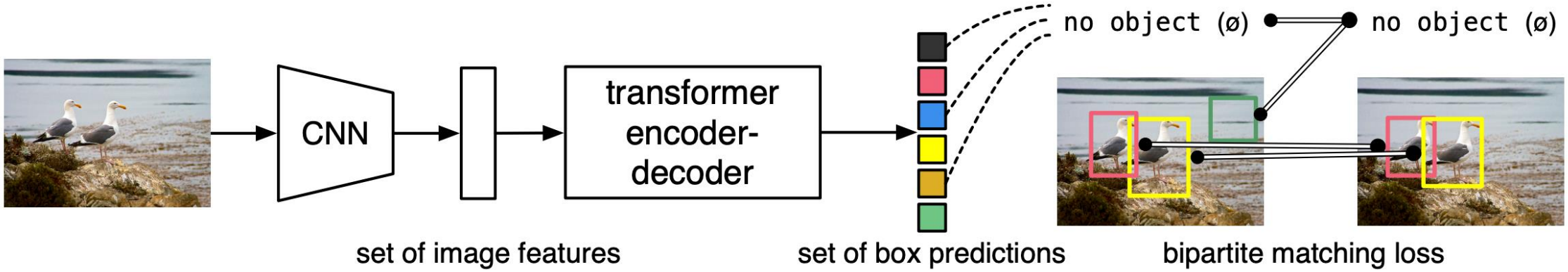
Chen et al, “CycleMLP: A MLP-like Architecture for Dense Prediction”, ICLR 2022, https://arxiv.org/abs/2107.10224

Object Detection with Transformers: DETR

Simple object detection pipeline: directly output a set of boxes from a Transformer

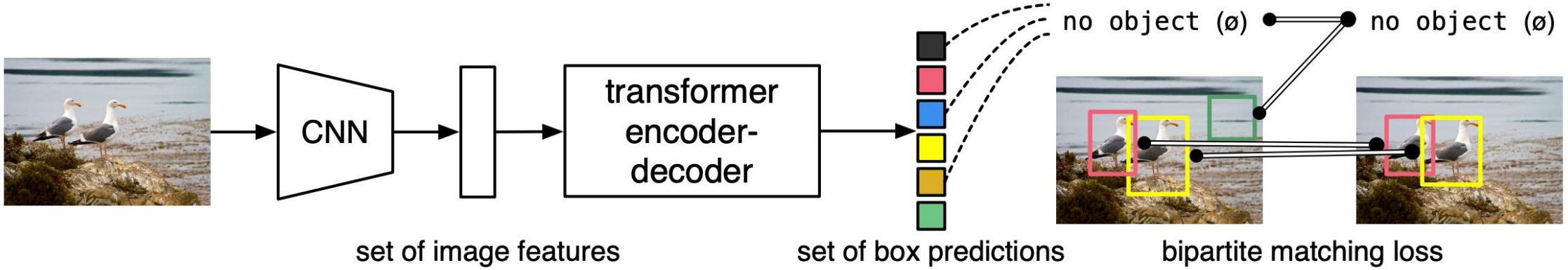
No anchors, no regression of box transforms

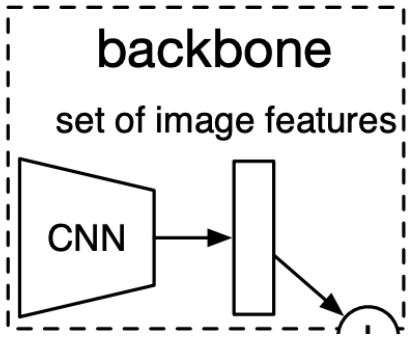
Match predicted boxes to GT boxes with bipartite matching; train to regress box coordinates



Carion et al, "End-to-End Object Detection with Transformers", ECCV 2020

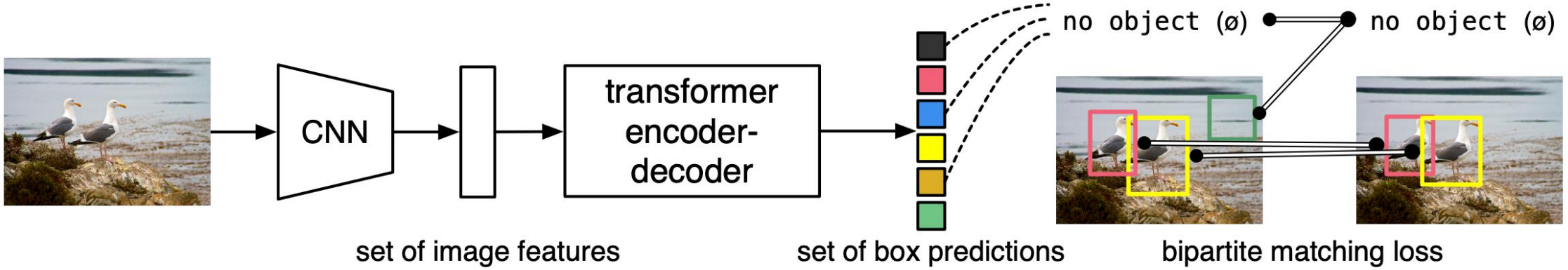
Object Detection with Transformers: DETR

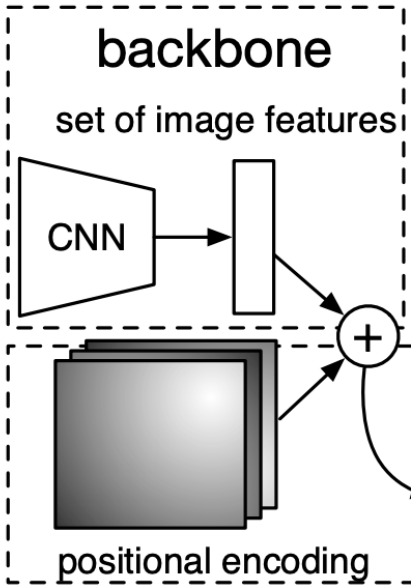




Carion et al, “End-to-End Object Detection with Transformers”, ECCV 2020

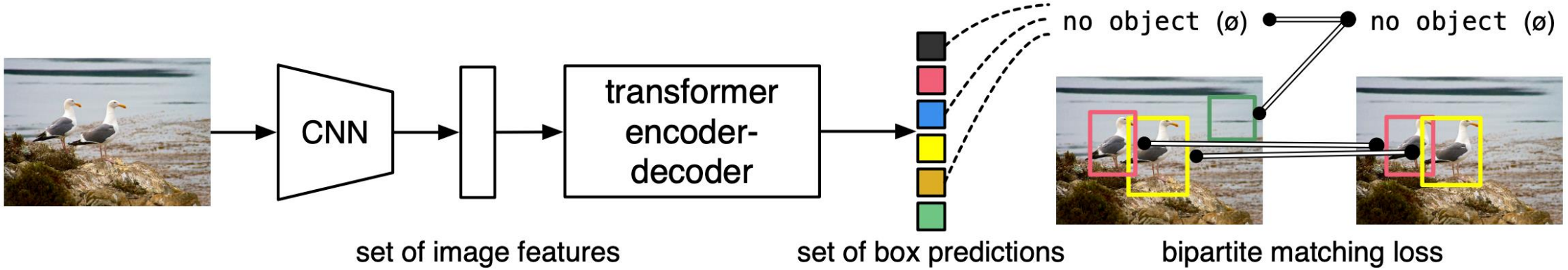
Object Detection with Transformers: DETR

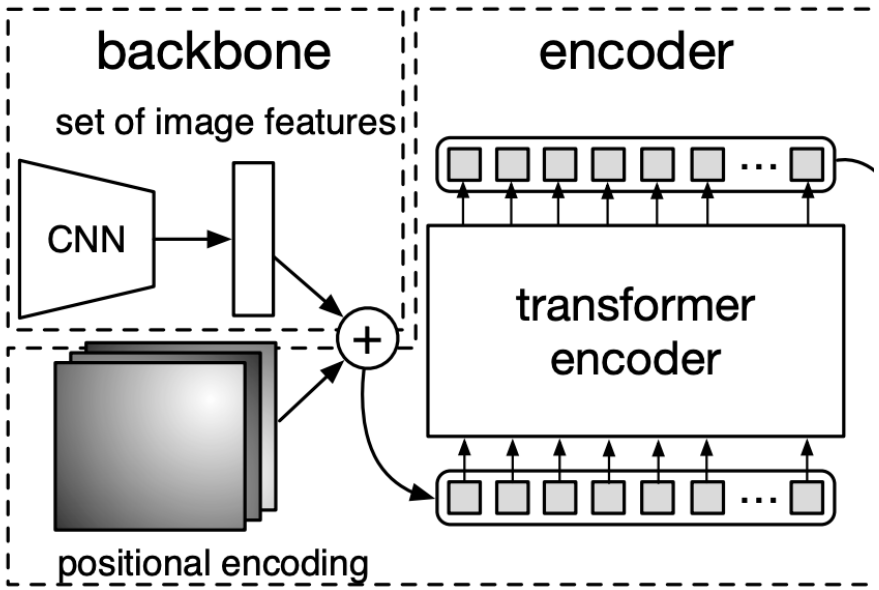




Carion et al, “End-to-End Object Detection with Transformers”, ECCV 2020

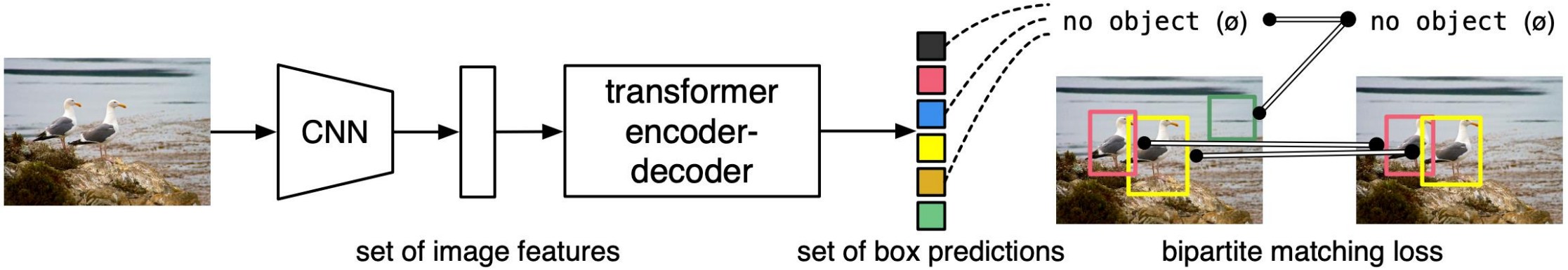
Object Detection with Transformers: DETR

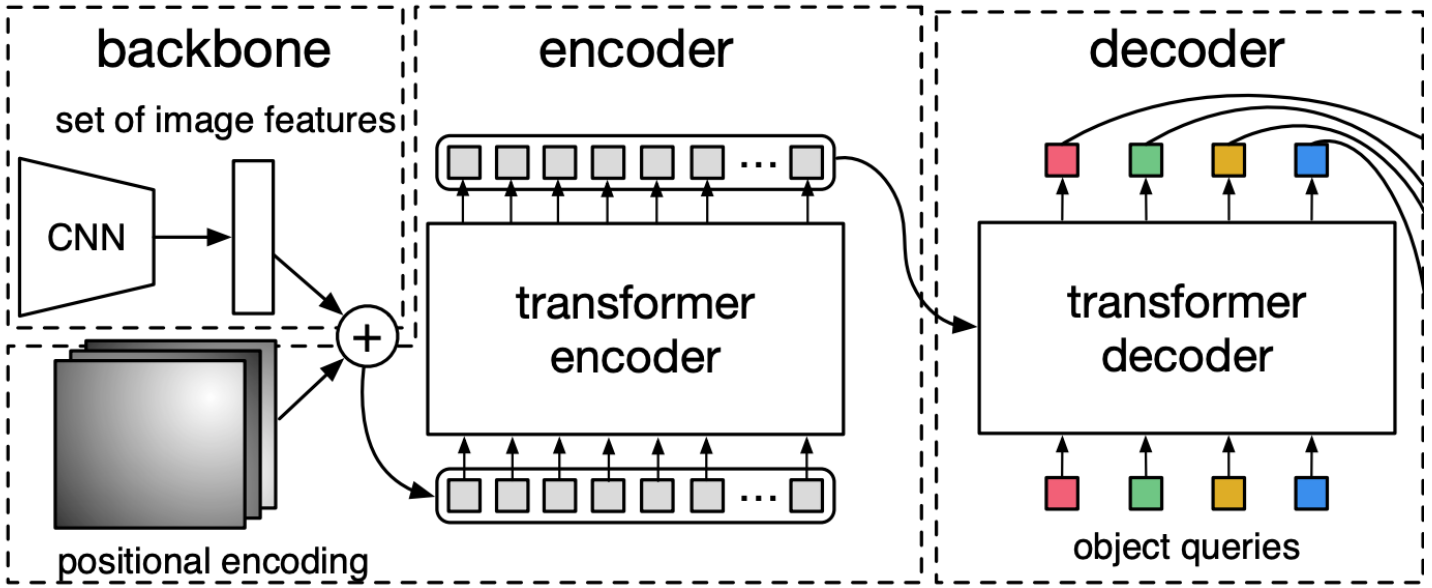




Carion et al, "End-to-End Object Detection with Transformers", ECCV 2020

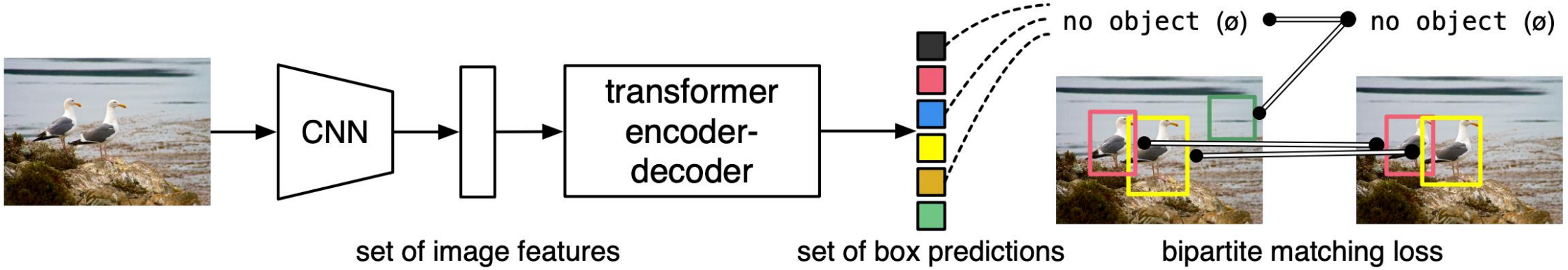
Object Detection with Transformers: DETR

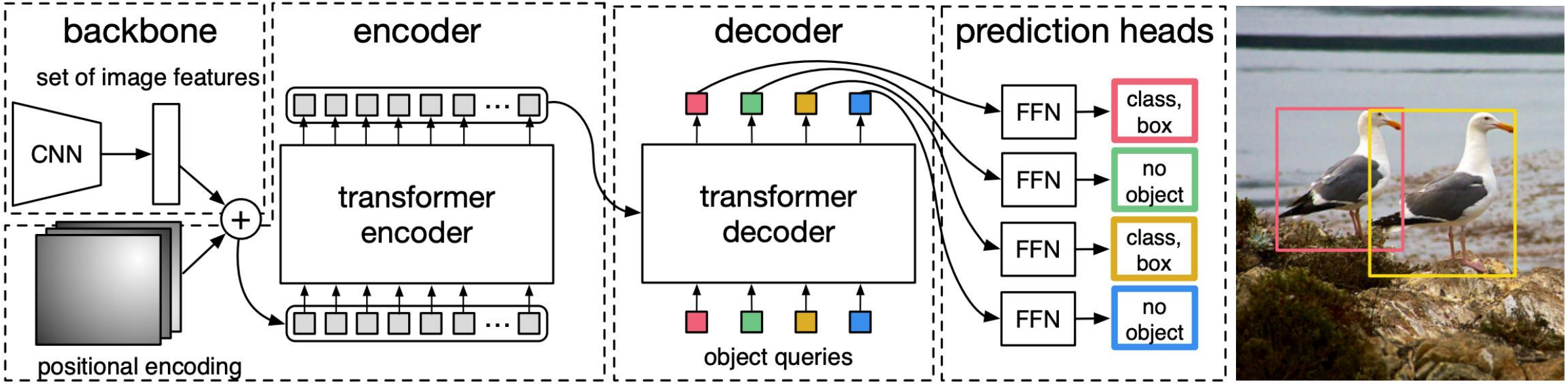




Carion et al, "End-to-End Object Detection with Transformers", ECCV 2020

Object Detection with Transformers: DETR





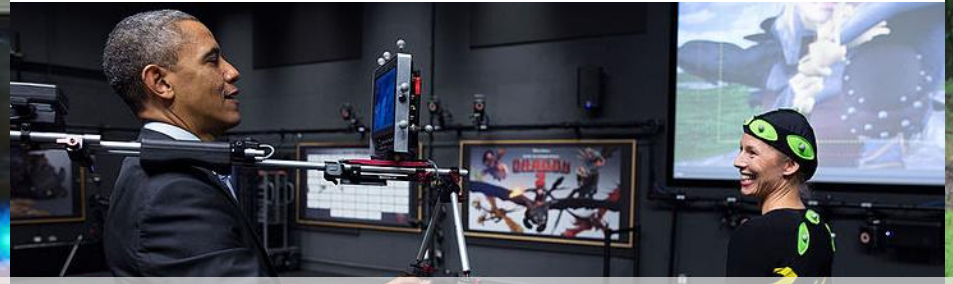
Carion et al, "End-to-End Object Detection with Transformers", ECCV 2020

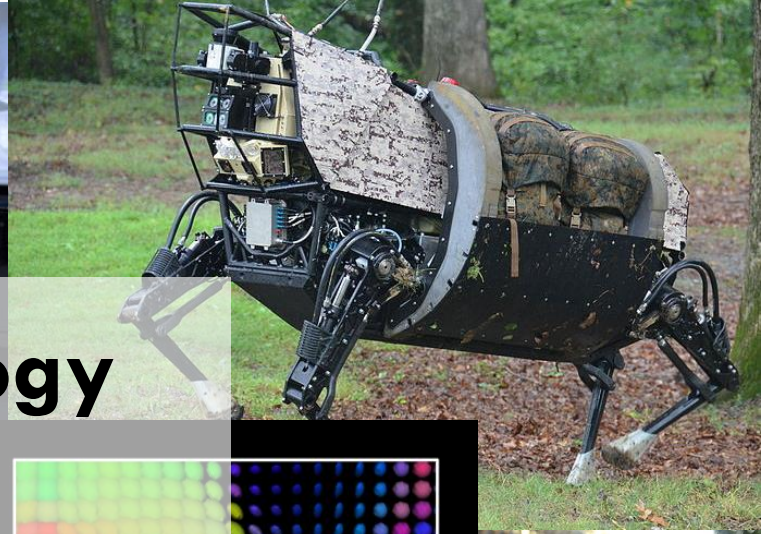
Vision Transformers Summary

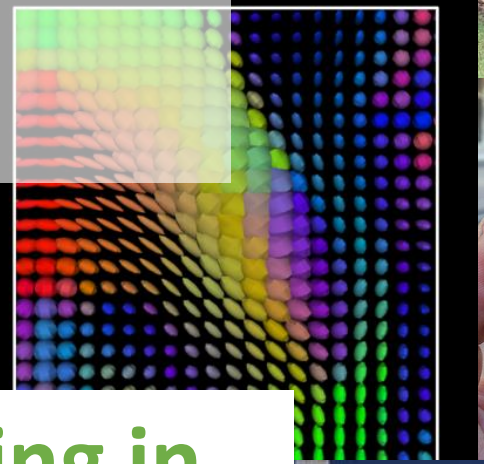
- ViTs have been a super hot topic the past ~1-2 years!
- Very different architecture vs. traditional CNNs
- Applications to all tasks: classification, detection, segmentation, etc.
- Vision Transformers are an evolution, not a revolution; we can still solve the same problems as with CNNs.
- Swin Transformer seems promising, but not the only state of the art
- Main benefit is probably speed: Matrix multiply is more hardware-friendly than convolution, so ViTs with same FLOPs as CNNs can train and run much faster

Computer Vision Technology

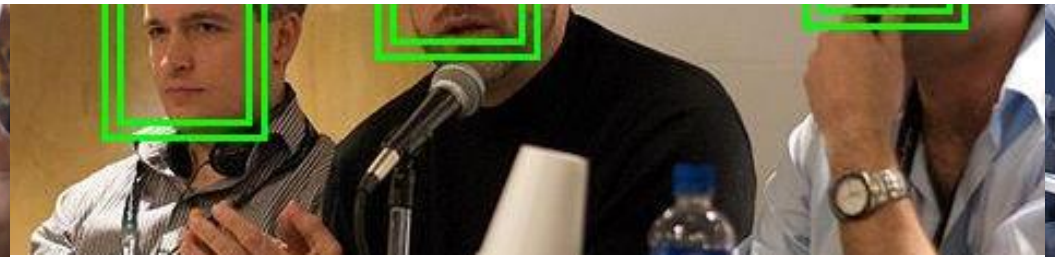
Can Better Our Lives







Now is a great time to be working in computer vision and machine learning!



The End!