24. Transformers STA3142 Statistical Machine Learning

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* Slides adapted from EECS498/598 @ Univ. of Michigan by Justin Johnson



The Rest of the Course Schedule

- 6/4 Tue: 22. Generative Models
- 6/6 Thu: 23. Recurrent Neural Networks (We have a class!)
- 6/9 Tue: 24. Transformers & 25. Reinforcement Learning
- **6/13 Thu**: 26. ML Advice
- 6/14 Fri: Final Assignment Deadline

Assignment 5 (Final Exam Replacement)

- Due Friday 6/14, 11:59pm
- Topic: Convolutional Neural Networks
 - Derive gradients for NN layers
 - Implement layers for CNNs
 - Train a CNN classifier for MNIST digit recognition
- Please read the instruction carefully!
 - Submit one pdf and one zip file separately
 - Write your code only in the designated spaces
 - Do not import additional libraries
 - ...
- If you feel difficult, consider to take option 2.

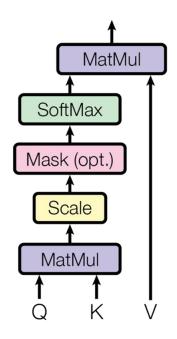
Attention

- Mapping a query and a set of key-value pairs to an output, where the query, keys, values, and output are all vectors
- Example: YouTube video search
 - Query: text prompt
 - Key: meta-information (video title, description, ...)
 - Value: videos
- Given a query, find the best matching key and return the corresponding value
 - Sort by matching scores in video search
 - Soft matching for attention mechanism
 - Return weighted sum of values; weights are normalized matching scores

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:



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

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

Inputs:

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

Computation:

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

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

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

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

Output vectors: Y = AV (Shape: $N_Q \times D_V$) $Y_i = \sum_i A_{i,i} V_i$

$$X_1$$





 Q_1



 Q_3

 Q_4

Inputs:

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

Computation:

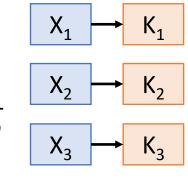
Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)

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

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

Attention weights: A = softmax(E, dim=1) (Shape: $N_0 \times N_X$)

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



 Q_1

 Q_2

 Q_3

 Q_4

Inputs:

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

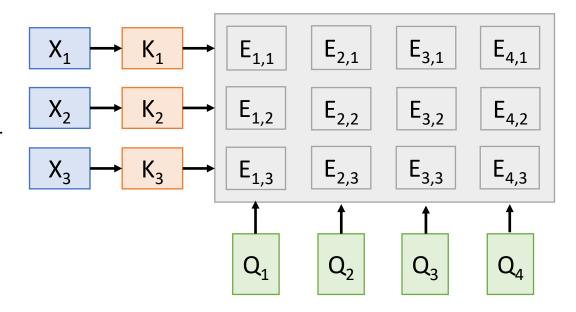
Computation:

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: $N_Q \times N_X$) $E_{i,j} = (Q_i \cdot K_j) / \sqrt{D_Q}$

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



Inputs:

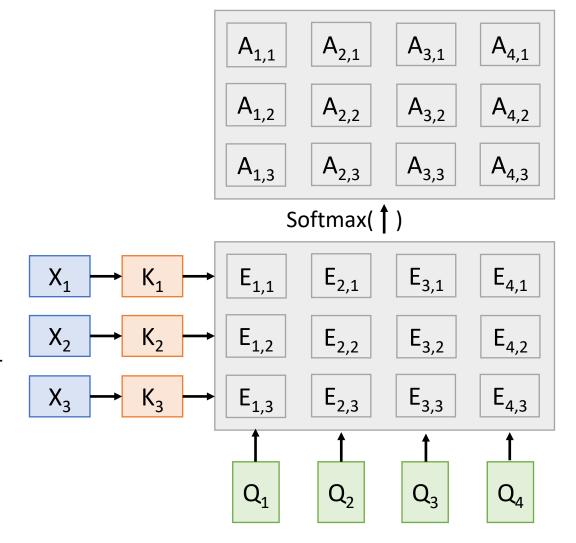
Query vectors: Q (Shape: $N_Q \times D_Q$) Input vectors: X (Shape: $N_X \times D_X$) Key matrix: W_K (Shape: $D_X \times D_Q$) Value matrix: W_V (Shape: $D_X \times D_V$)

Computation:

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: $N_Q \times N_X$) $E_{i,j} = (Q_i \cdot K_i) / \sqrt{D_Q}$

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



Inputs:

Query vectors: \mathbf{Q} (Shape: $N_0 \times D_0$) **Input vectors**: X (Shape: $N_x \times D_x$) **Key matrix**: W_{κ} (Shape: $D_{x} \times D_{0}$) Value matrix: W_v (Shape: $D_x \times D_v$)

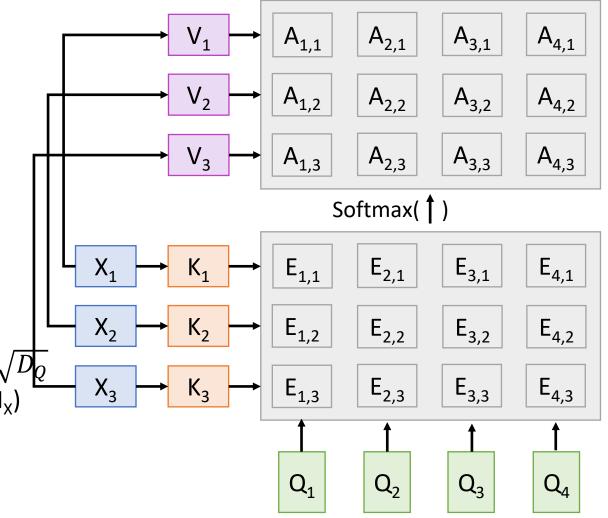
Computation:

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

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

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

Attention weights: A = softmax(E, dim=1) (Shape: $N_0 \times N_x$)



Inputs:

Query vectors: \mathbf{Q} (Shape: $N_0 \times D_0$) **Input vectors**: X (Shape: $N_x \times D_x$) **Key matrix**: W_{κ} (Shape: $D_{x} \times D_{0}$) Value matrix: W_v (Shape: $D_x \times D_v$)

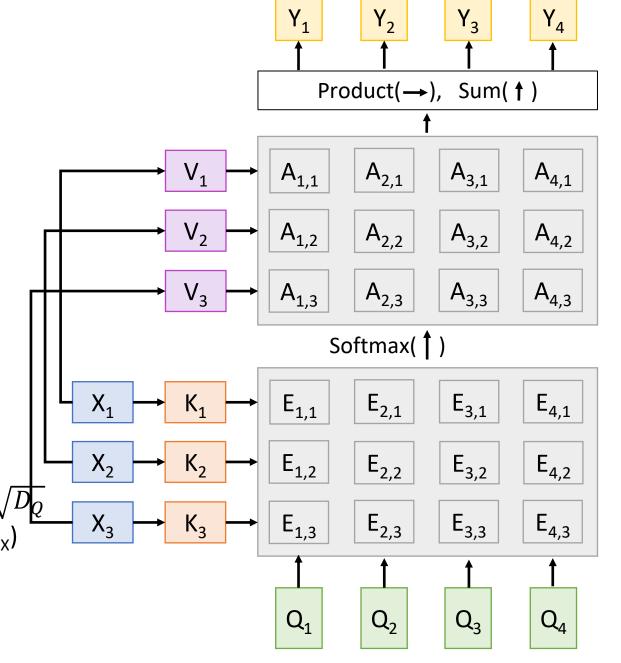
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Key vectors: $K = XW_K$ (Shape: $N_X \times D_O$)

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

Attention weights: A = softmax(E, dim=1) (Shape: $N_0 \times N_x$)



One query per input vector

Inputs:

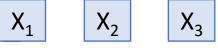
Query vectors: Q (Shape: $N_Q \times D_Q$) Input vectors: X (Shape: $N_X \times D_X$) Key matrix: W_K (Shape: $D_X \times D_Q$) Value matrix: W_V (Shape: $D_X \times D_V$)

Computation:

Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$) Value Vectors: $V = XW_V$ (Shape: $N_X \times D_V$)

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

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



One query per input vector

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_O (Shape: $D_X \times D_O$)

Computation:

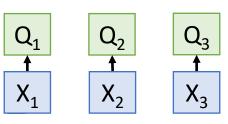
Query vectors: Q = XW_o

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

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

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

Attention weights: A = softmax(E, dim=1) (Shape: $N_x \times N_x$)



One query per input vector

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_O (Shape: $D_X \times D_Q$)

Computation:

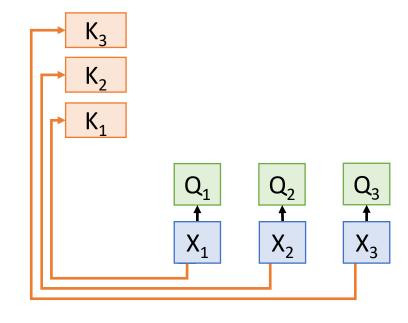
Query vectors: Q = XW_o

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

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

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

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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_O (Shape: $D_X \times D_Q$)

Computation:

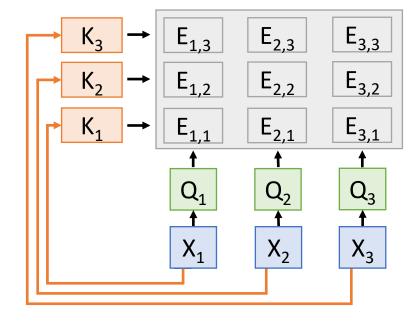
Query vectors: $Q = XW_Q$

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

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

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One query per input vector

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_O (Shape: $D_X \times D_Q$)

Computation:

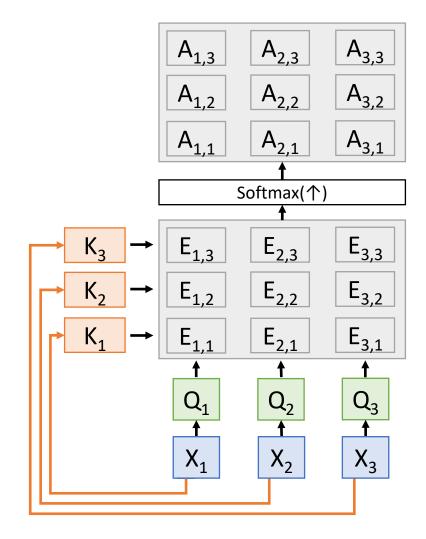
Query vectors: Q = XW_Q

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

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

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One query per input vector

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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_O (Shape: $D_X \times D_O$)

Computation:

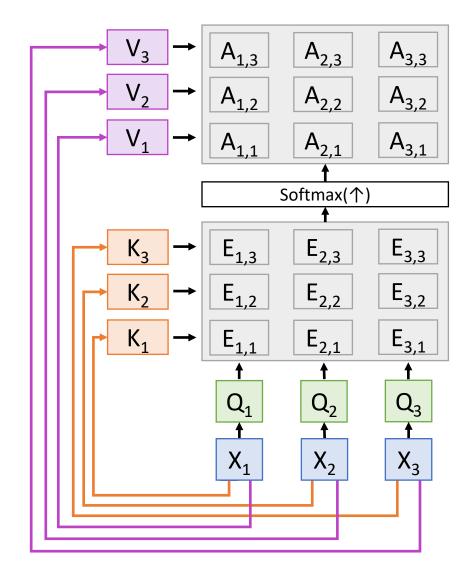
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Key vectors: $K = XW_K$ (Shape: $N_X \times D_Q$)

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One query per input vector

Inputs:

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Computation:

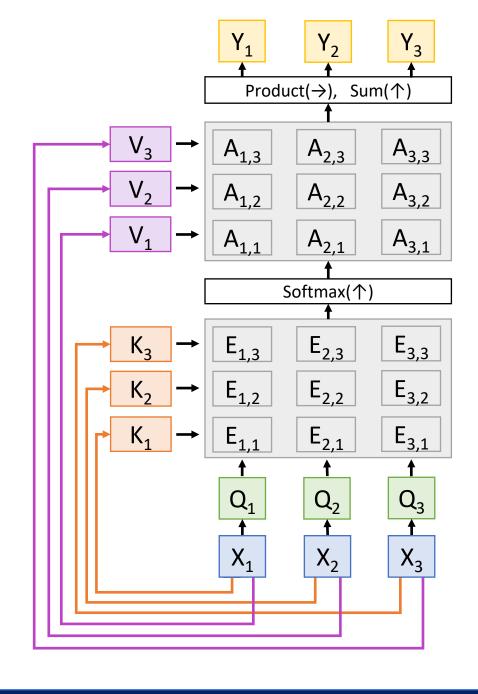
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Attention weights: A = softmax(E, dim=1) (Shape: $N_X \times N_X$)



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_O (Shape: $D_X \times D_O$)

Computation:

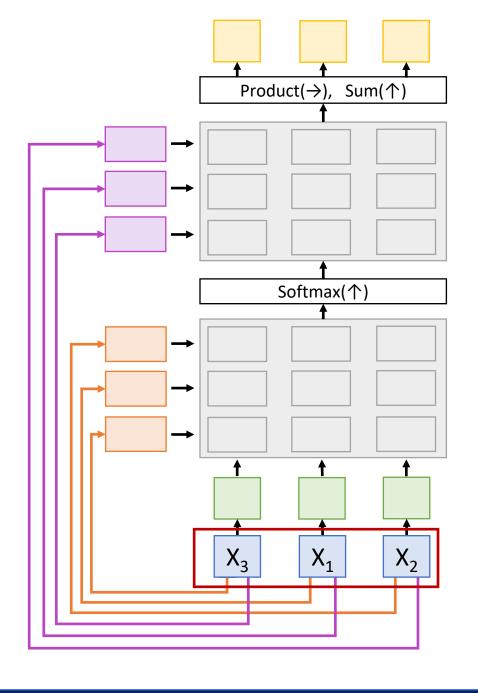
Query vectors: Q = XW_Q

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

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

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

Attention weights: A = softmax(E, dim=1) (Shape: $N_x \times N_x$)



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: $D_X \times D_Q$)

Queries and Keys will be the same, but permuted

Computation:

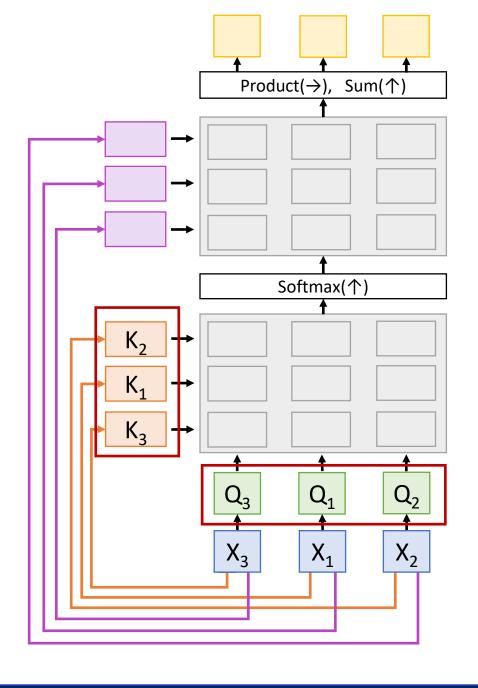
Query vectors: $Q = XW_0$

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

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

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

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



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: $D_X \times D_Q$)

Similarities will be the same, but permuted

Computation:

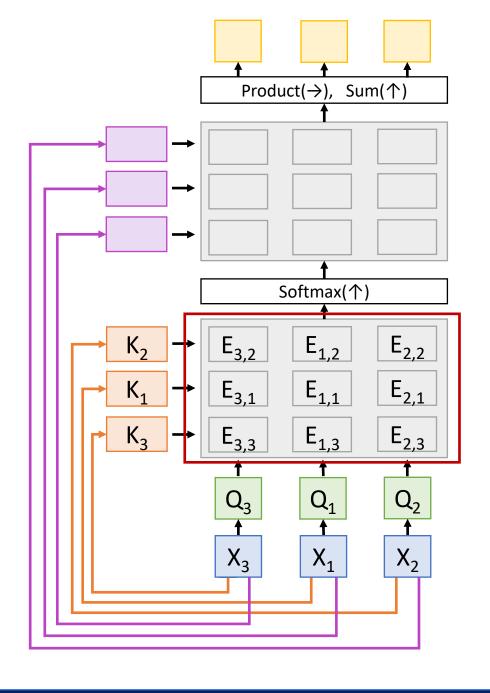
Query vectors: $Q = XW_0$

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

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

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

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



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: $D_X \times D_Q$)

Attention weights will be the same, but permuted

Computation:

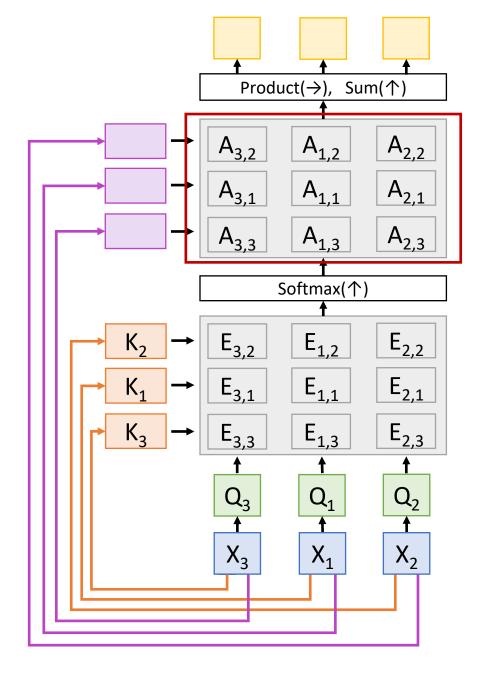
Query vectors: $Q = XW_Q$

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

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

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

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



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: $D_X \times D_Q$)

Values will be the same, but permuted

Computation:

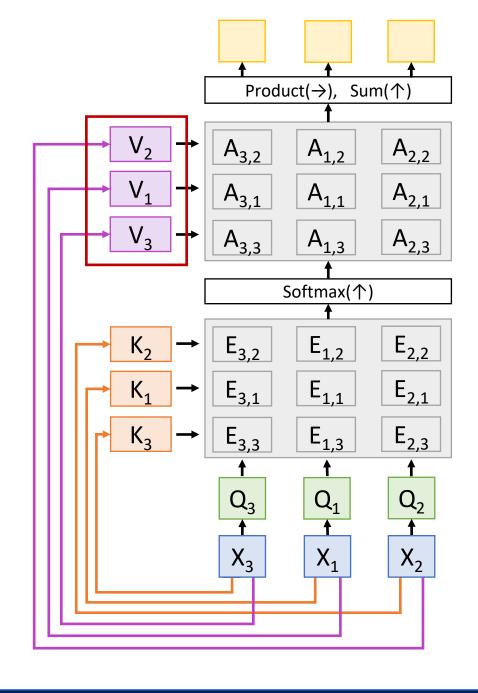
Query vectors: $Q = XW_0$

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

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

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

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



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

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

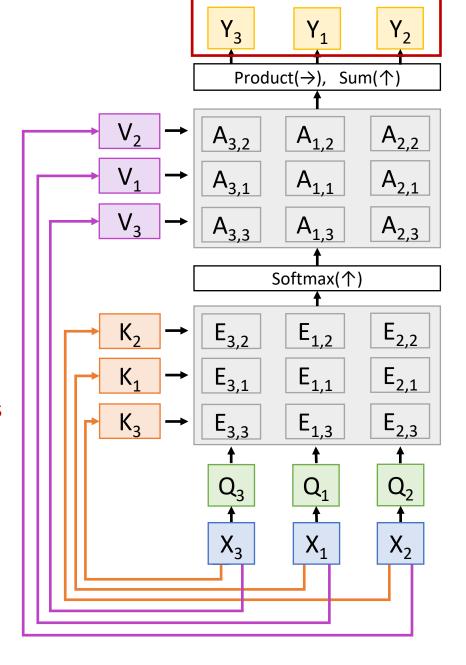
Output vectors: Y = AV (Shape: $N_X \times D_V$) $Y_i = \sum_j A_{i,j} V_j$

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

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_O (Shape: $D_X \times D_Q$)

Computation:

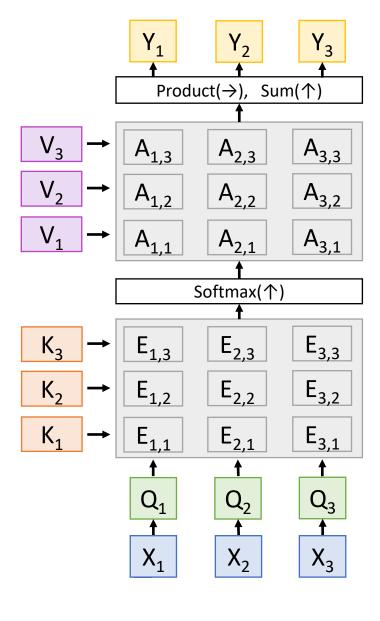
Query vectors: $Q = XW_Q$

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

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

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

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



Inputs:

Input vectors: X (Shape: $N_x \times D_x$) **Key matrix**: W_{κ} (Shape: $D_{\chi} \times D_{\Omega}$) Value matrix: W_v (Shape: $D_x \times D_v$) Query matrix: W_0 (Shape: $D_x \times D_0$) Self attention doesn't "know" the order of the vectors it is processing!

In order to make processing positionaware, concatenate or add positional encoding to the input

Computation:

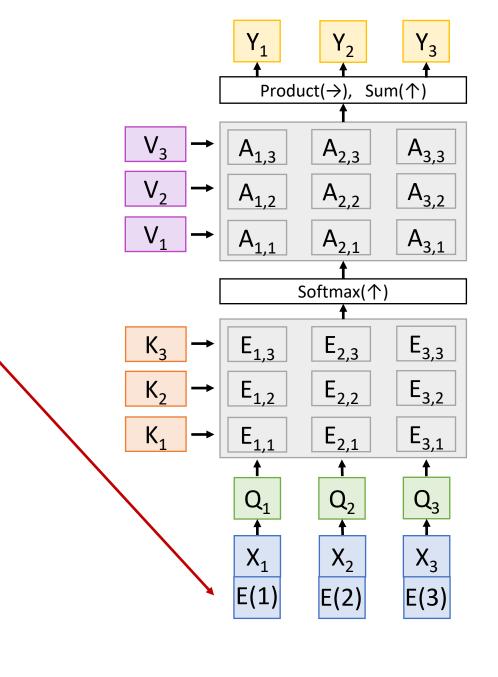
Query vectors: $Q = XW_0$

E is either learnable or **Key vectors**: $K = XW_K$ (Shape: $N_X \times D_O$) fixed (sinusoidal wave)

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

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

Attention weights: A = softmax(E, dim=1) (Shape: $N_x \times N_x$)



Masked Self-Attention Layer

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

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_0 (Shape: $D_x \times D_0$)

Computation:

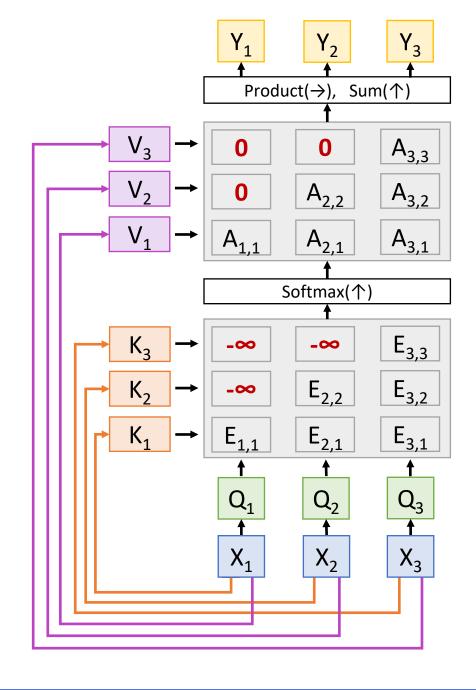
Query vectors: Q = XW_o

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

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

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

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



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: $N_X \times D_X$) 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:

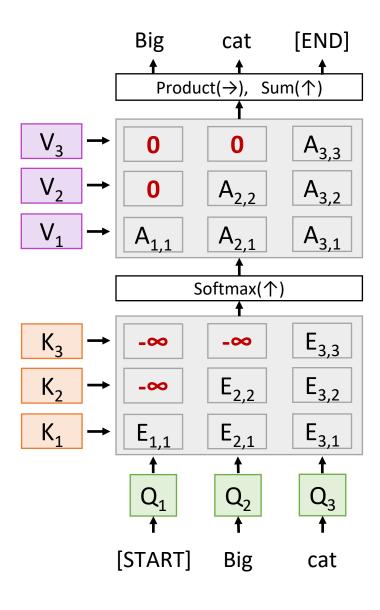
Query vectors: Q = XW_Q

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

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

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

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



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_o

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

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

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

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

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

 X_1

X₂

X

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: $E = \mathbf{Q}\mathbf{K}^{\mathsf{T}} / \sqrt{D_Q}$ (Shape: $N_X \times N_X$) $E_{i,j} = (\mathbf{Q}_i \cdot \mathbf{K}_j) / \sqrt{D_Q}$

Attention weights: A = softmax(E, dim=1) (Shape: $N_x \times N_x$)

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

 $X_{1,1}$ $X_{1,2}$ $X_{1,3}$

Split

X_{2,1}
X_{2,2}
X_{2,3}

X_{3,1}
X_{3,2}
X_{3,3}

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

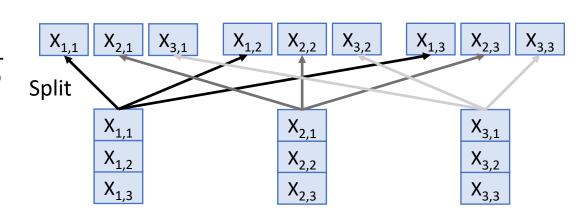
Computation:

Query vectors: $Q = XW_Q$

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Attention weights: A = softmax(E, dim=1) (Shape: $N_x \times N_x$)



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:

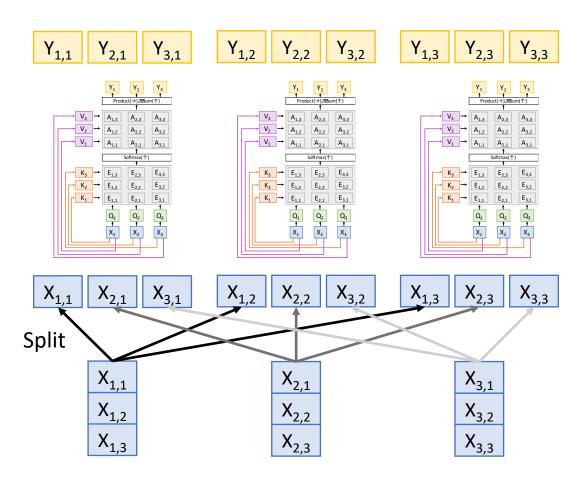
Query vectors: Q = XW_Q

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

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

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

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



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

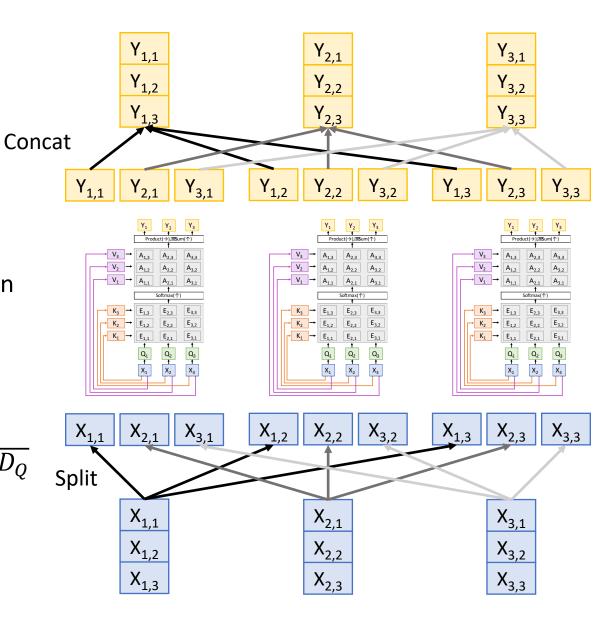
Computation:

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

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



<u>Inputs</u>:

Input vectors: X (Shape: $N_X \times D_X$) Key matrix: W_K (Shape: $D_X \times D_O$)

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:

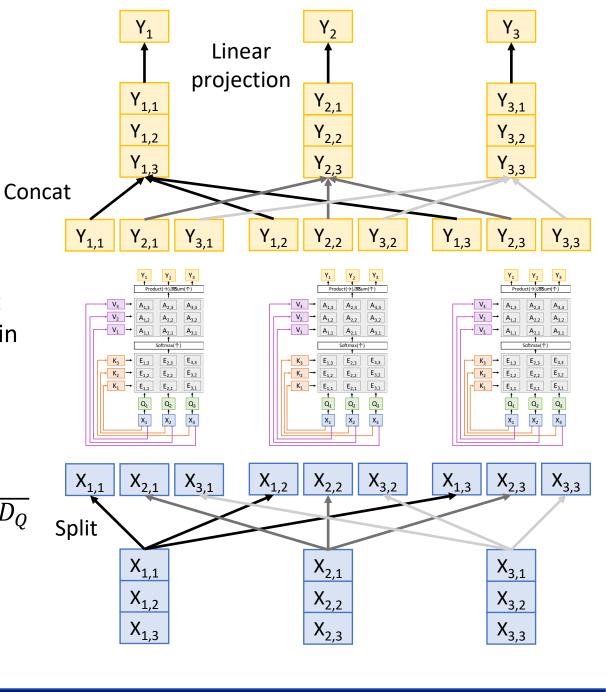
Query vectors: $Q = XW_Q$

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

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

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

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



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.

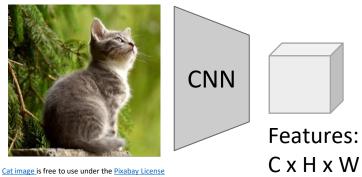
Multi-Head Attention is defined as:

$$MultiHead(Q, K, V) = Concat(head_1, ..., head_h)W^O$$

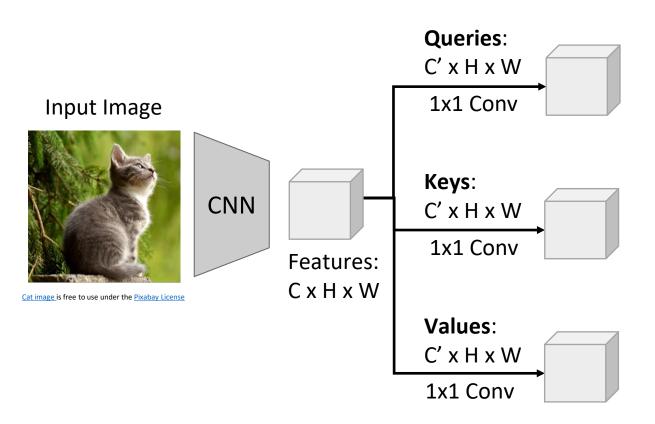
where $head_i = Attention(QW_i^Q, KW_i^K, VW_i^V)$.

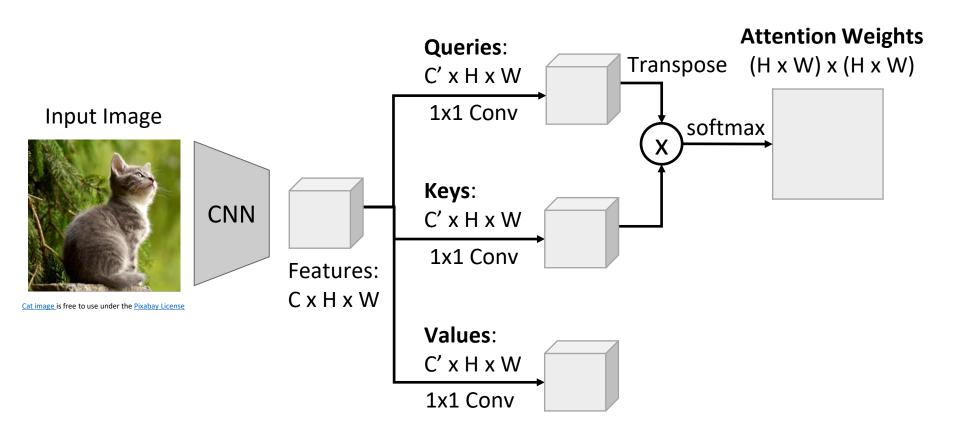
Example: CNN with Self-Attention

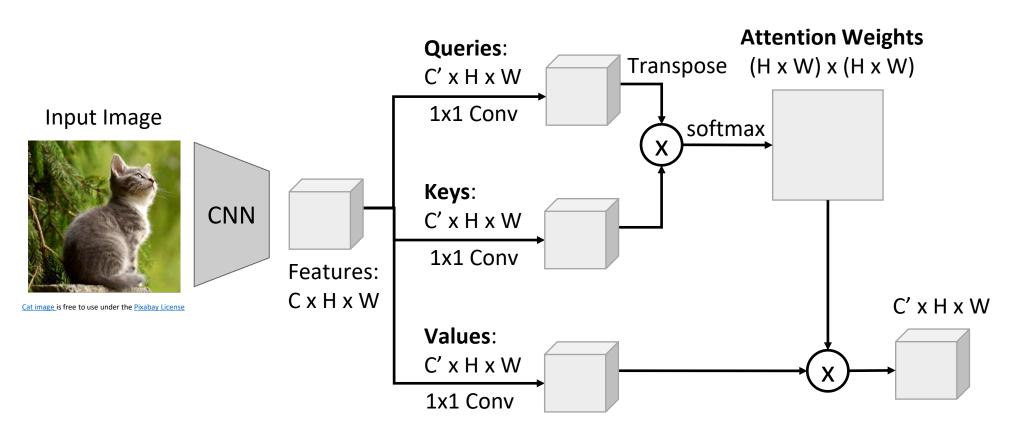
Input Image

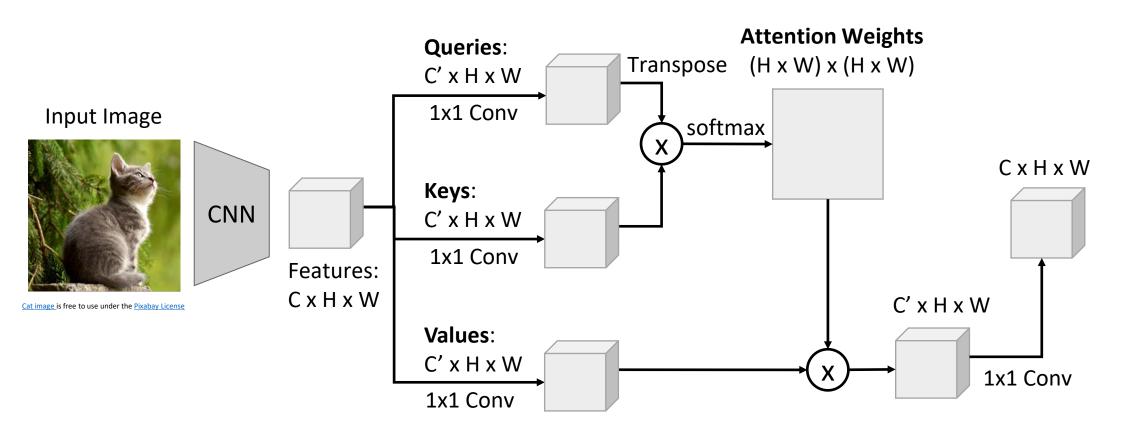


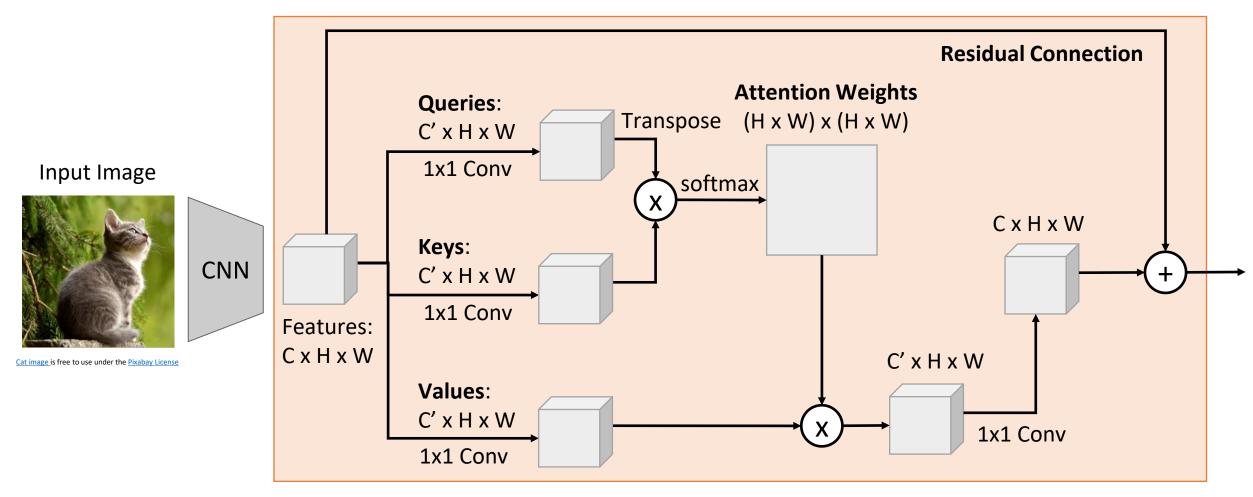
Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2018





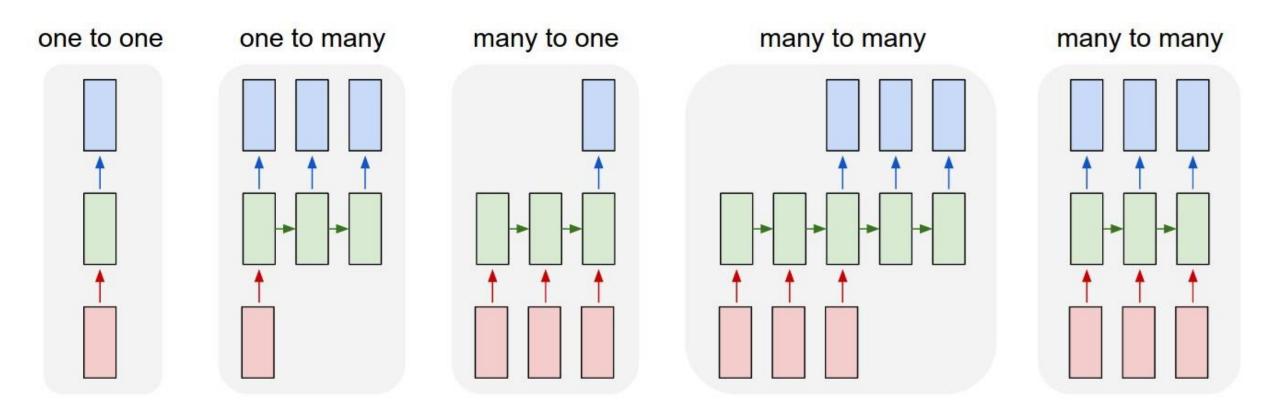






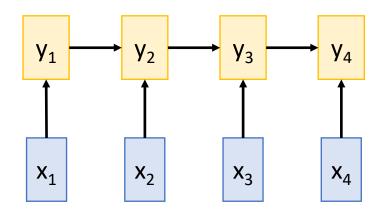
Self-Attention Module

Recall: Recurrent Neural Networks

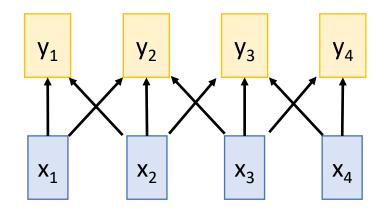


Three Ways of Processing Sequences

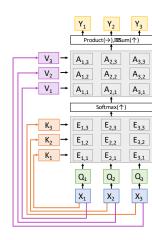
Recurrent Neural Network



1D Convolution



Self-Attention



Works on **Ordered Sequences**

- (+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence
- (-) Not parallelizable: need to compute hidden states sequentially

Works on Multidimensional Grids

- (-) Bad at long sequences: Need to stack many conv layers for outputs to "see" the whole sequence
- (+) Highly parallel: Each output can be computed in parallel

Works on **Sets of Vectors**

- (-) Good at long sequences: after one self-attention layer, each output "sees" all inputs!
- (+) Highly parallel: Each output can be computed in parallel
- (-) Very memory intensive

Three Ways of Processing Sequences

Recurrent Neural Network

1D Convolution

Self-Attention

Attention is all you need

Vaswani et al, NeurIPS 2017

Works on **Ordered Sequences**

- (+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence
- (-) Not parallelizable: need to compute hidden states sequentially

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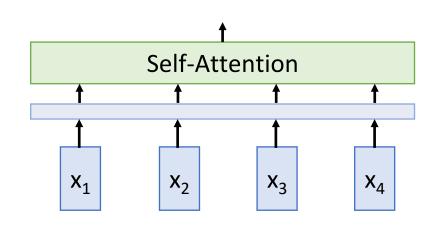
X₁

 X_2

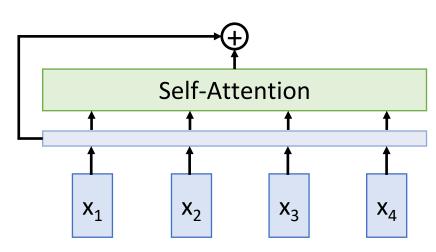
X₃

 X_4

All vectors interact with each other



Residual connection
All vectors interact
with each other



Recall Layer Normalization:

Given $h_1, ..., h_N$ (Shape: D)

scale: γ (Shape: D)

shift: β (Shape: D)

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

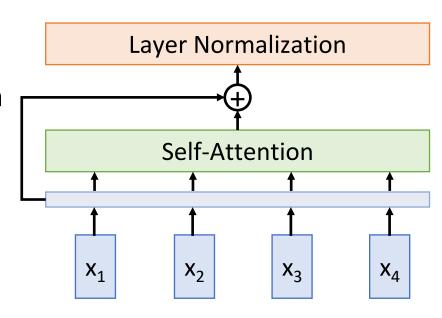
$$\sigma_{i} = (\sum_{i} (h_{i,i} - \mu_{i})^{2}/D)^{1/2}$$
 (scalar)

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

$$y_i = \gamma * z_i + \beta$$

Ba et al, 2016

Residual connection
All vectors interact
with each other



Recall Layer Normalization:

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scale: γ (Shape: D)

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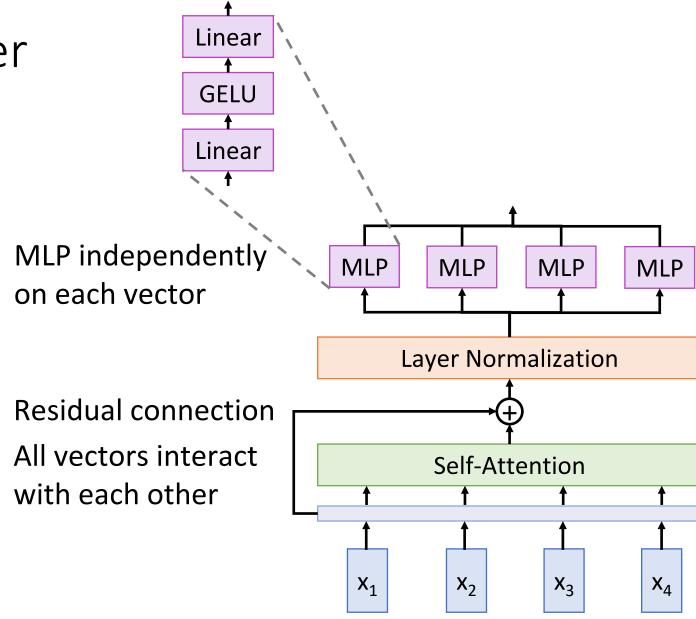
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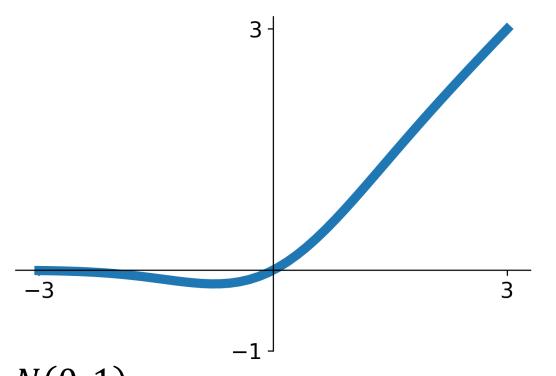
$$z_i = (h_i - \mu_i) / \sigma_i$$

$$y_i = \gamma * z_i + \beta$$

Ba et al, 2016



Activation Function: Gaussian Error Linear Unit (GELU)



$$X \sim N(0, 1)$$

$$gelu(x) = xP(X \le x) = \frac{x}{2} (1 + \text{erf}(x/\sqrt{2}))$$

$$\approx x\sigma(1.702x)$$

- Idea: Multiply input by 0 or 1 at random; large values more likely to be multiplied by 1, small values more likely to be multiplied by 0 (data-dependent dropout)
- Take expectation over randomness
 - Very common in Transformers (BERT, GPT, ViT)
- Cf. Swish (or SiLU): $x\sigma(x)$

Hendrycks and Gimpel, Gaussian Error Linear Units (GELUs), 2016 Ramachandran et al, Swish: a Self-Gated Activation Function, 2017

Recall Layer Normalization:

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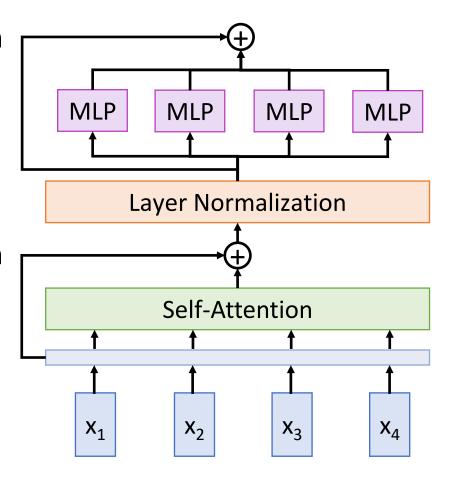
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Ba et al, 2016

Residual connection

MLP independently on each vector

Residual connection
All vectors interact
with each other



Recall Layer Normalization:

Given $h_1, ..., h_N$ (Shape: D)

scale: γ (Shape: D)

shift: β (Shape: D)

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

 $\sigma_{i} = (\sum_{i} (h_{i,i} - \mu_{i})^{2}/D)^{1/2}$ (scalar)

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

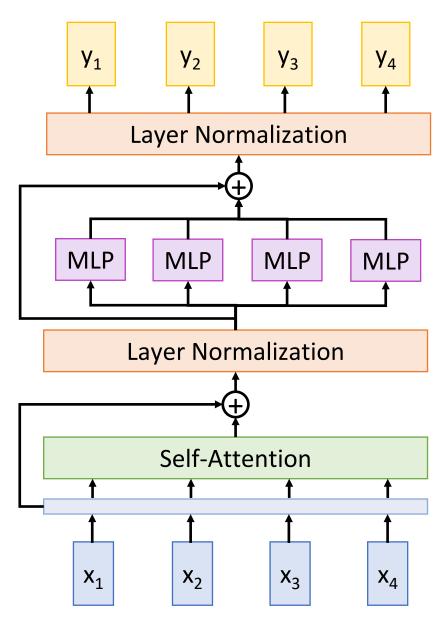
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Ba et al, 2016

Residual connection

MLP independently on each vector

Residual connection
All vectors interact
with each other



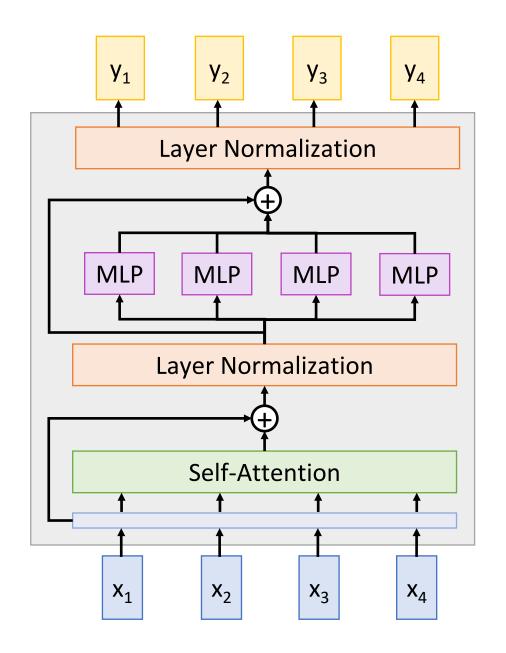
Transformer Block:

Input: Set of vectors x

Output: Set of vectors y

Hyperparameters:

- Number of blocks
- Number of heads per block
- Width (channels per head, FFN width)



Transformer Block:

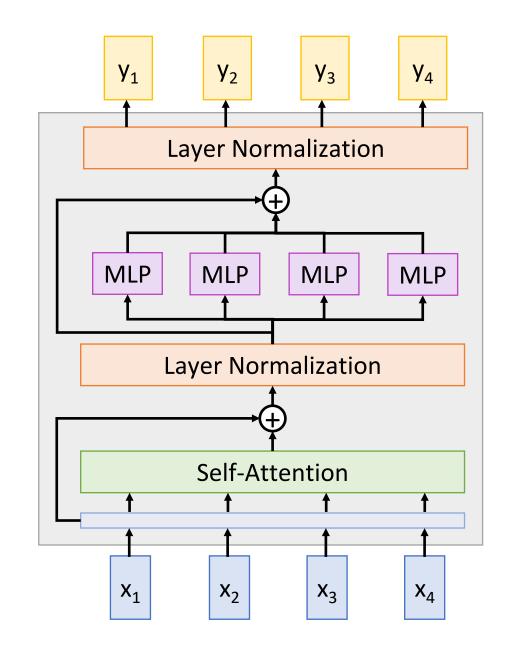
Input: Set of vectors x

Output: Set of vectors y

Self-attention is the only interaction between vectors!

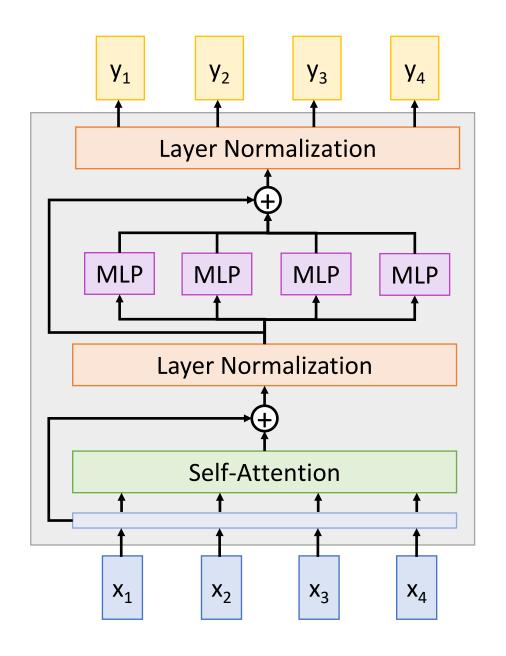
Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable



Post-Norm Transformer

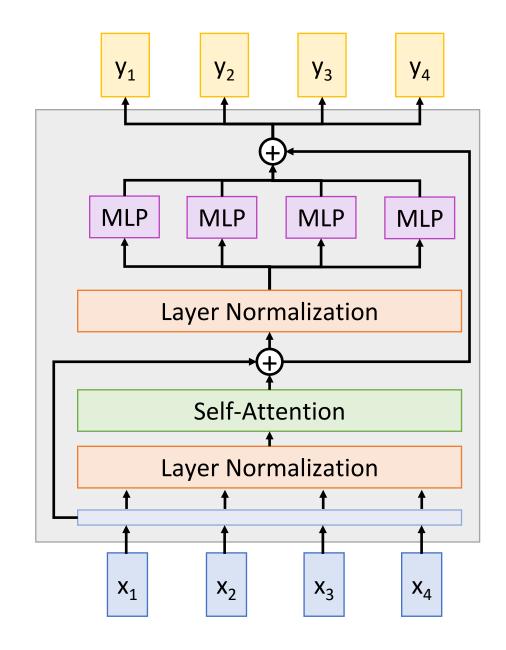
Layer normalization is after residual connections



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

Transformer Block:

Input: Set of vectors x

Output: Set of vectors y

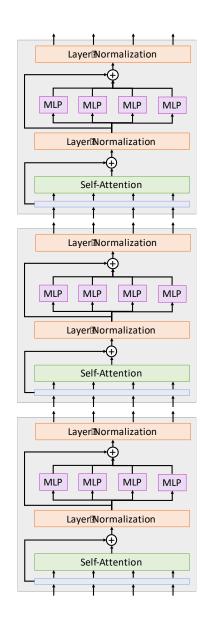
Self-attention is the only interaction between vectors!

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_o=512, 6 heads



The Transformer: Transfer Learning

"ImageNet Moment for Natural Language Processing"

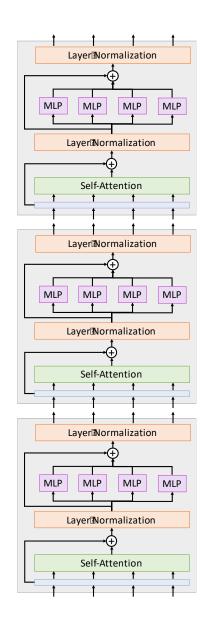
Pre-training:

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



Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M		8x P100 (12 hours)
Transformer-Large	12	1024	16	213M		8x P100 (3.5 days)

Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M		8x P100 (12 hours)
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BERT-Base	12	768	12	110M	13 GB	
BERT-Large	24	1024	16	340M	13 GB	

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

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RoBERTa	24	1024	16	355M	160 GB	1024x V100 GPU (1 day)

Yang et al, XLNet: Generalized Autoregressive Pretraining for Language Understanding", 2019 Liu et al, "RoBERTa: A Robustly Optimized BERT Pretraining Approach", 2019

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\$3,768,320 on Google Cloud (eval price)

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Rae et al, "Scaling Language Models: Methods, Analysis, & Insights from Training Gopher", arXiv 2021

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PaLM	118	18,432	256	540B	?	6144x TPUv4 (38 days)

Chowdhery et al, "PaLM: Scaling Language Modeling with Pathways", arXiv 2022

Specifications are veiled!

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GPT-3	96	12,288	96	175B	694 GB	?
Gopher	80	16,384	128	280B	10.55 TB	4096x TPUv3 (38 days)
PaLM	118	18,432	256	540B	?	6144x TPUv4 (38 days)
GPT-4	?	?	?	? (1T?)	?	?

OpenAI, "GPT-4 Technical Report", arXiv 2023

Specifications are veiled!

Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M		8x P100 (12 hours)
Transformer-Large	12	1024	16	213M		8x P100 (3.5 days)
BERT-Base	12	768	12	110M	13 GB	
BERT-Large	24	1024	16	340M	13 GB	
XLNet-Large	24	1024	16	~340M	126 GB	512x TPU-v3 (2.5 days)
RoBERTa	24	1024	16	355M	160 GB	1024x V100 GPU (1 day)
GPT-2	48	1600	?	1.5B	40 GB	
Megatron-LM	72	3072	32	8.3B	174 GB	512x V100 GPU (9 days)
Turing-NLG	78	4256	28	17B	?	256x V100 GPU
GPT-3	96	12,288	96	175B	694 GB	?
Gopher	80	16,384	128	280B	10.55 TB	4096x TPUv3 (38 days)
PaLM	118	18,432	256	540B	?	6144x TPUv4 (38 days)
GPT-4	?	?	,	? (1T?)	?	?
PaLM 2	?	?	?	?	?	?

Generated Text from GPT-3

Bold text: Input prompt written by humans

Italics: Completion by GPT-3

Title: United Methodists Agree to Historic Split

Subtitle: Those who oppose gay marriage will form their own denomination

Article:

Generated Text from GPT-3

Bold text: Input prompt written by humans

Italics: Completion by GPT-3

Title: United Methodists Agree to Historic Split

Subtitle: Those who oppose gay marriage will form their own denomination

Article: After two days of intense debate, the United Methodist Church has agreed to a historic split - one that is expected to end in the creation of a new denomination, one that will be "theologically and socially conservative," according to The Washington Post. The majority of delegates attending the church's annual General Conference in May voted to strengthen a ban on the ordination of LGBTQ clergy and to write new rules that will "discipline" clergy who officiate at same-sex weddings. But those who opposed these measures have a new plan: They say they will form a separate denomination by 2020, calling their church the Christian Methodist denomination. The Post notes that the denomination, which claims 12.5 million members, was in the early 20th century the "largest Protestant denomination in the U.S.," but that it has been shrinking in recent decades. The new split will be the second in the church's history. The first occurred in 1968, when roughly 10 percent of the denomination left to form the Evangelical United Brethren Church. The Post notes that the proposed split "comes at a critical time for the church, which has been losing members for years," which has been "pushed toward the brink of a schism over the role of LGBTQ people in the church." Gay marriage is not the only issue that has divided the church. In 2016, the denomination was split over ordination of transgender clergy, with the North Pacific regional conference voting to ban them from serving as clergy, and the South Pacific regional conference voting to allow them.

GPT-3: Programming by prompt

Bold text: Input prompt written by humans

Italics: Completion by GPT-3

Poor English input: I eated the purple berries.

Good English output: I ate the purple berries.

Poor English input: Thank you for picking me as your designer. I'd appreciate it.

Good English output: Thank you for choosing me as your designer. I appreciate it.

Poor English input: The mentioned changes have done. or I did the alteration that you

requested. or I changed things you wanted and did the modifications.

Good English output: The requested changes have been made. or I made the alteration

that you requested. or I changed things you wanted and made the modifications.

Poor English input: I'd be more than happy to work with you in another project.

Good English output:

GPT-3: Programming by prompt

Input / Output examples
Test example

Italics: Completion by GPT-3

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Topic: humor: literary parodies and homages, pastiches, style parodies.

Parodies of the fantasy novel series *Harry Potter* in the style of various famous authors:

By Ernest Hemingway:

"It was a cold day on Privet Drive. A child cried. Harry felt nothing.

Topic: humor: literary parodies and homages, pastiches, style parodies.

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By Ernest Hemingway:

"It was a cold day on Privet Drive. A child cried. Harry felt nothing. He was dryer than dust. He had been silent too long. He had not felt love. He had scarcely felt hate. Yet the Dementor's Kiss killed nothing. Death didn't leave him less dead than he had been a second before. It wasn't about living or dying really. It wasn't about death. It was about the Dark Lord, his creator, his engenderer. He was not resurrected. He was created again. He was whole again in the courtyard of Malfoy Manor."

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By Jane Austen:

"It is a truth universally acknowledged, that a broken Harry is in want of a book. This he knows to his cost; pressing that wretched nose against the window of a bookstore in Diagon Alley the last thing before he goes into hiding for several years, where upon, he goes straight to Azkaban."

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By Arthur Conan Doyle:

"Harry pushed at the swinging doors of the bookshop hard, and nearly knocked himself unconscious. He staggered in with his ungainly package, his cheeks scarlet with cold and the shame of having chosen the wrong month to go Christmas shopping. The proprietor of the store, however, didn't cast even a cursory glance at him, being far more interested in an enormous hunk of wood lying in the middle of the floor, which certainly looked like a gallows. Yes, the proprietor said to a reedy old man wearing a bowler hat and a forlorn expression that made Harry want to kick him, I can rent you such a gallows for a small fee."

ChatGPT: Artificial Intelligence Chatbot

◆[†] Model: GPT-4



What does ChatGPT can do?



How long will it take to reach artificial general intelligence?



ChatGPT, like me, is an artificial intelligence model developed by OpenAI. It's a language model, which means it's been trained on a vast amount of text data to be able to generate human-like text based on given input. Here's an overview of what ChatGPT can do:



- 2. **Text completion and generation:** If you provide the beginning of a story or a sentence, ChatGPT can complete it in a coherent and contextually appropriate manner.
- 3. **Conversational partner:** ChatGPT can have engaging conversations on a wide range of topics. It can act as a chatbot for various purposes.
- 4. **Tutoring:** ChatGPT can provide explanations and tutorials on many topics, particularly academic ones such as mathematics, physics, philosophy, history, etc.
- 5. **Brainstorming and idea generation:** ChatGPT can generate ideas, suggestions, and help in brainstorming sessions.
- 6. **Language translation:** While not its primary function, ChatGPT can perform simple translations.
- 7. **Writing assistance:** ChatGPT can help in drafting emails, writing essays, creating content, and other writing tasks.
- 8. **Role-playing scenarios:** ChatGPT can be used in simulations or role-play exercises, playing a specific character or role.



As of my last training data in September 2021, it's impossible to provide a precise timeline for the development of Artificial General Intelligence (AGI), the point at which artificial intelligence would be able to understand, learn, and apply knowledge across a broad array of tasks at a level equal to or beyond that of a human being. Predicting the arrival of AGI is a challenging task due to the numerous scientific and technical hurdles that need to be overcome.

Researchers and experts in the field of artificial intelligence have a range of opinions on when AGI might be achieved, with some predicting it could happen within a few decades, while others believe it could take a century or more, or even that it might not be achievable at all.

It's also important to note that the development of AGI would raise significant ethical, societal, and safety issues. For instance, if AGI surpasses human intelligence, there could be profound implications for society, including questions about control, purpose, and the potential displacement of humans in many areas of work and life.

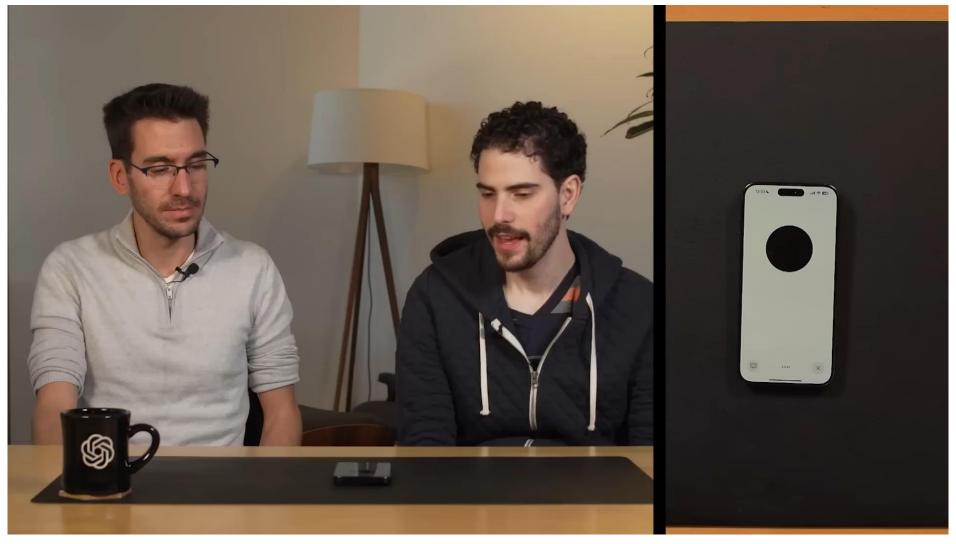
As of now, a significant amount of research is being conducted on these topics, and any responsible development of AGI should take these considerations into account. It's recommended to keep an eye on the latest research and consensus among experts in the field for the most up-to-date predictions and discussions regarding AGI.

GPT-40: Reasoning across audio, vision, and text



https://www.youtube.com/watch?v=vgYi3Wr7v_g

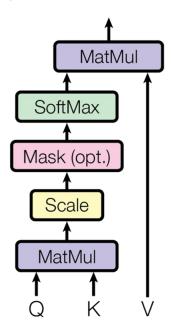
GPT-40: Realtime translation



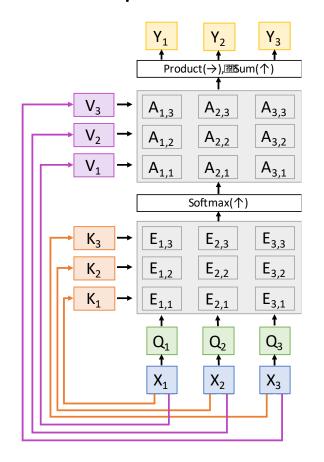
https://www.youtube.com/watch?v=WzUnEfilqP4

Summary

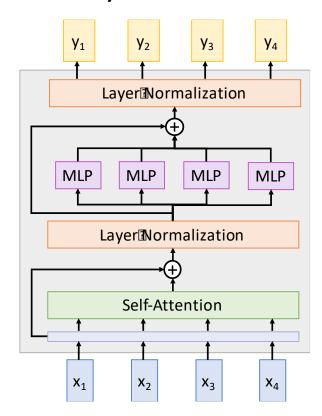
Attention mechanism: mapping a query and a set of key-value pairs to an output (= attention map)



Generalized **Self-Attention** is new, powerful neural network primitive



Transformers are a new neural network model that only uses attention



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

Next: Reinforcement Learning