CAP 5516 Medical Image Computing (Spring 2025)

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Lecture 8: Introduction to Deep Learning (3)

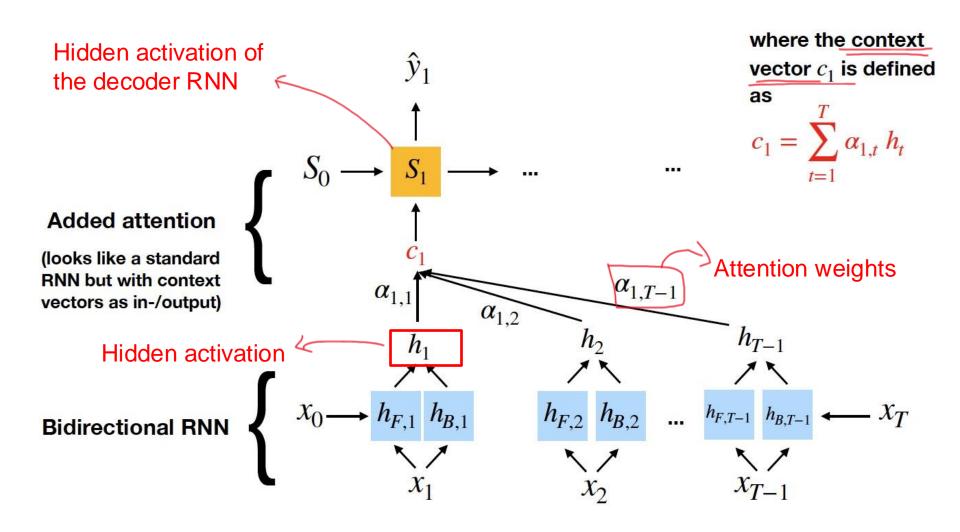


Attention Mechanism

- The attention mechanism is a technique used to selectively focus on the most relevant parts of an input, rather than using the entire input equally, when producing a prediction.
- It allows a network to dynamically weigh the importance of different elements in the input and focus on the most relevant ones when making a decision.
- The attention mechanism has proven to be particularly effective in tasks such as machine translation and image captioning, where a model must consider different parts of an input when making a prediction.

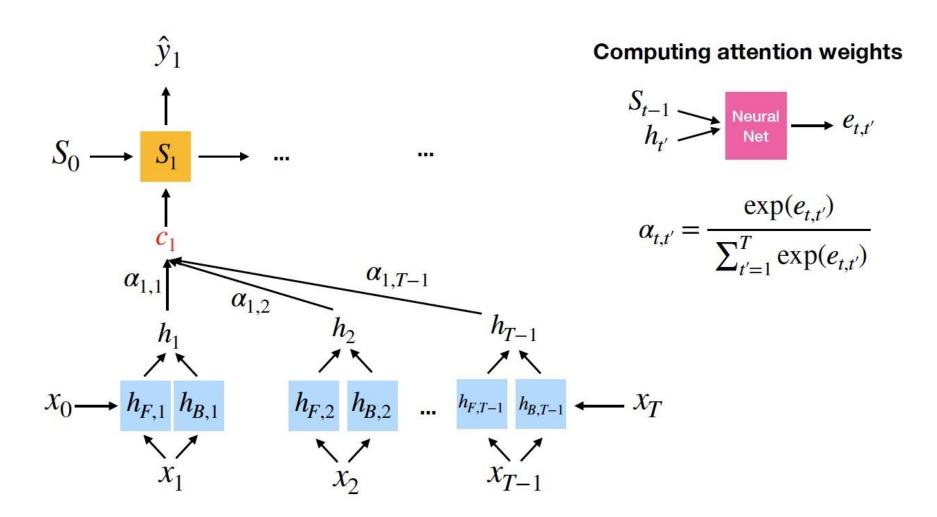


RNN with Attention Mechanism



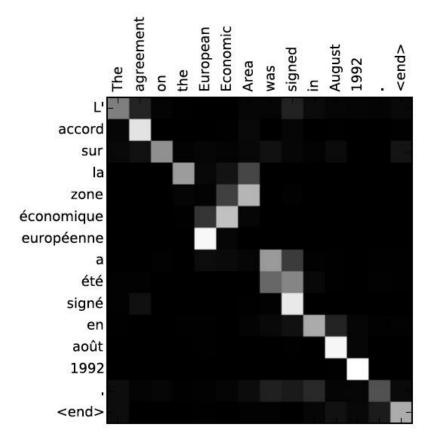


RNN with Attention Mechanism





RNN with Attention Mechanism



Computing attention weights

$$\begin{array}{c} S_{t-1} \\ h_{t'} \end{array} \longrightarrow \begin{array}{c} \text{Neural} \\ \text{Net} \end{array} \longrightarrow e_{t,t'}$$

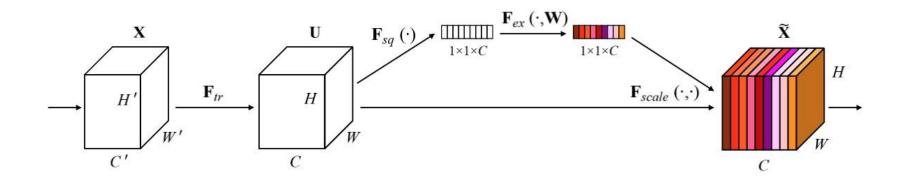
$$\alpha_{t,t'} = \frac{\exp(e_{t,t'})}{\sum_{t'=1}^{T} \exp(e_{t,t'})}$$

Figure: Bahdanau, D., Cho, K., & Bengio, Y. (2014). Neural machine translation by jointly learning to align and translate. https://arxiv.org/abs/1409.0473



Attention in CNNs

Squeeze-and-Excitation Networks

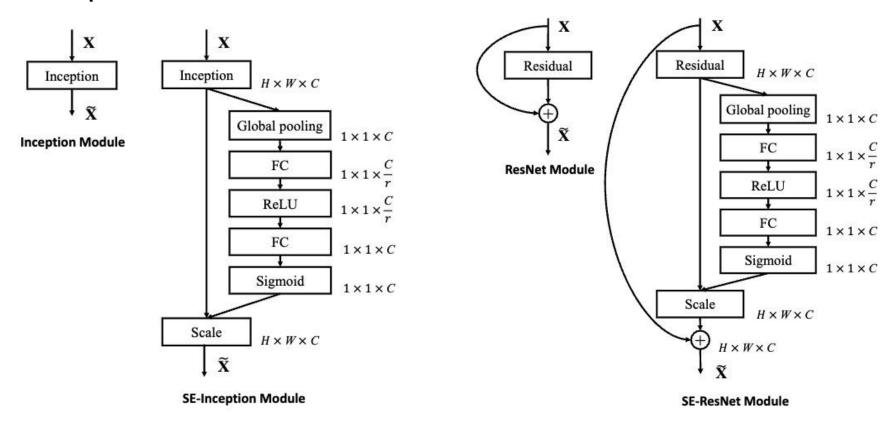


Hu, J., Shen, L., & Sun, G. (2018). Squeeze-and-excitation networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 7132-7141).



Attention in CNNs

Squeeze-and-Excitation Networks



Hu, J., Shen, L., & Sun, G. (2018). Squeeze-and-excitation networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 7132-7141).



Transformer



Attention Is All You Need

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Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. In Advances in neural information processing systems (pp. 5998-6008).

https://arxiv.org/abs/1706.03762

Attention is all you need

A Vaswani, N Shazeer, N Parmar... - Advances in neural ..., 2017 - proceedings.neurips.cc

... to attend to all positions in the decoder up to and including that position. We need to prevent

... We implement this inside of scaled dot-product attention by masking out (setting to -∞) ...

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Since ~2018, Transformers have been growing in popularity ... and size

GPT-3 (175B parameters)

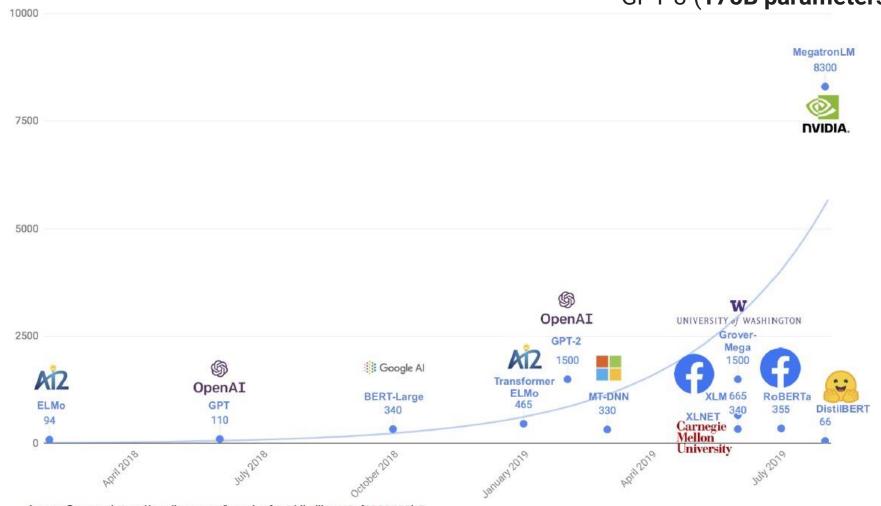
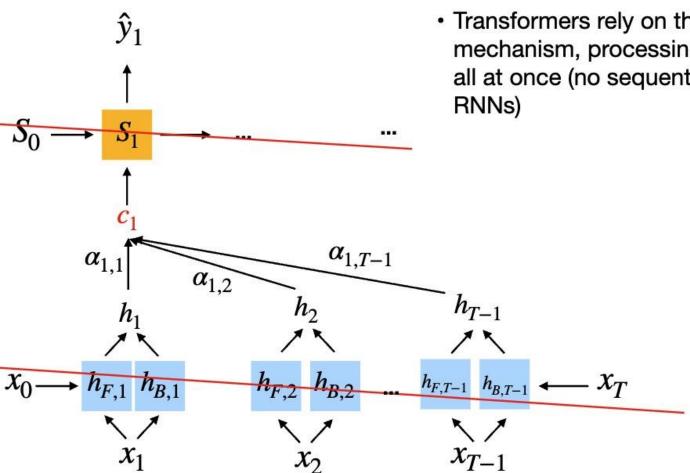


Image Source: https://medium.com/huggingface/distilbert-8cf3380435b5



Getting rid of the sequential parts



 Transformers rely on the self-attention mechanism, processing the whole sequence all at once (no sequential processing like in

12

Self-Attention Mechanism -- Very Basic Form

Main procedure:

- Derive attention <u>weights</u>: similarity between current input and all other inputs (next slide)
- 2) Normalize weights via softmax (next slide)
- Compute attention value from normalized weights and corresponding inputs (below)

Self-attention as weighted sum:

$$A_i = \sum_{j=1}^T a_{ij} x_j$$

output corresponding to the i-th input

weight based on similarity between current input x_i and all other inputs

Self-Attention Mechanism -- Very Basic Form

Self-attention as weighted sum:

 $A_i = \sum_{j=1}^{I} a_{ij} x_j$

output corresponding to the i-th input

weight based on similarity between current input x_i and all other inputs

How to compute the attention weights?

here as simple dot product:

$$e_{ij} = \boldsymbol{x}_i^{\top} \boldsymbol{x}_j$$

repeat this for all inputs $j \in \{1...T\}$, then normalize

$$a_{ij} = \frac{\exp\left(e_{ij}\right)}{\sum_{j=1}^{T} \exp\left(e_{ij}\right)} = \operatorname{softmax}\left(\left[e_{ij}\right]_{j=1....T}\right)$$

Self-Attention Mechanism -- Very Basic Form

a. B = || all | 1 bil cost

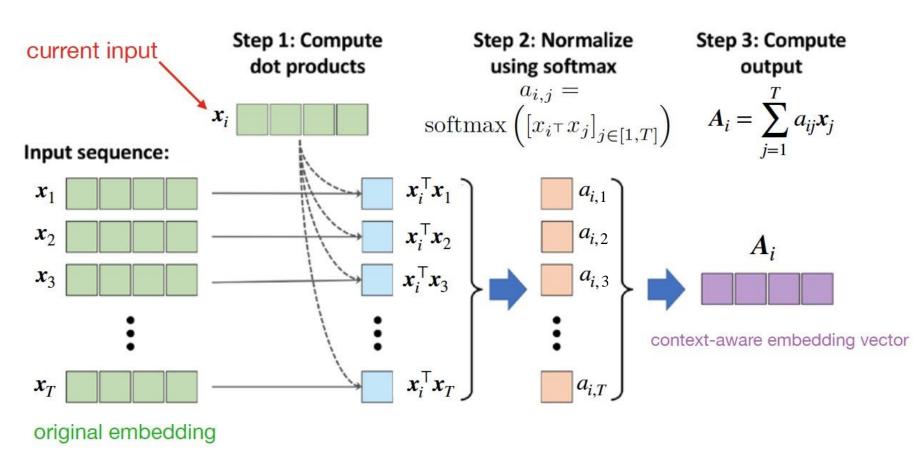


Image source: Raschka & Mirjalili 2019. Python Machine Learning, 3rd edition

Attention Is All You Need

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Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. In *Advances in neural information processing systems* (pp. 5998-6008).

https://arxiv.org/abs/1706.03762



- Previous basic version did not involve any learnable parameters, so not very useful for learning a language model
- We are now adding 3 trainable weight matrices that are multiplied with the input sequence embeddings (x_i) 's)

query =
$$W^q x_i$$

key = $W^k x_i$
value = $W^v x_i$



1. Query:

 In the transformer, the query vector corresponds to the feature representation of the current token (or position) that is "asking" how much it should attend to other tokens in the input sequence.

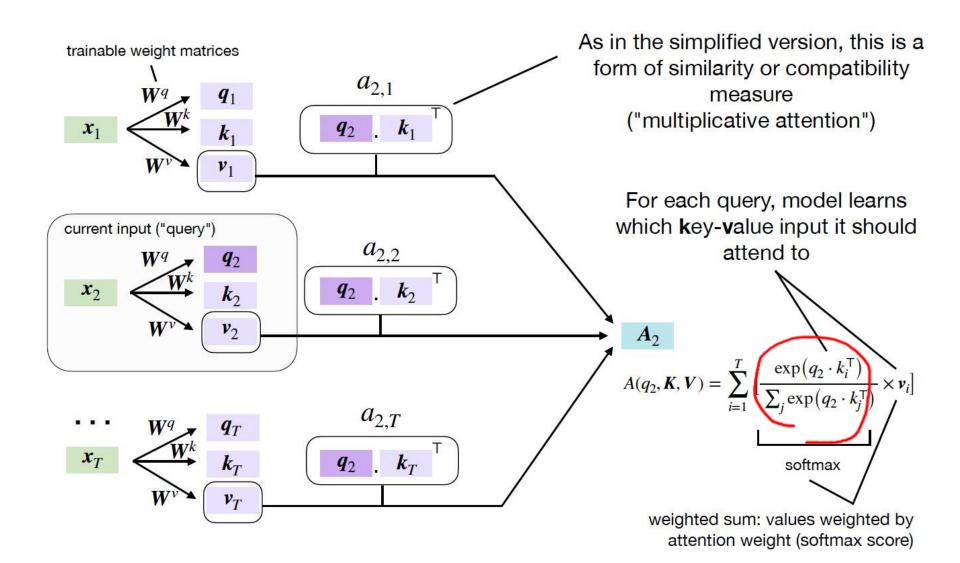
2. **Key**:

 In the transformer, the key vector represents the features of a token (or position) in the sequence. It is used in conjunction with the query to determine the degree of relevance or attention between tokens.

3. Value:

 In the transformer, the value vector represents the actual feature content of a token (or position). Once attention weights are calculated using the query and key, these weights are applied to the value vectors to compute the weighted sum, which represents the output of the attention mechanism.



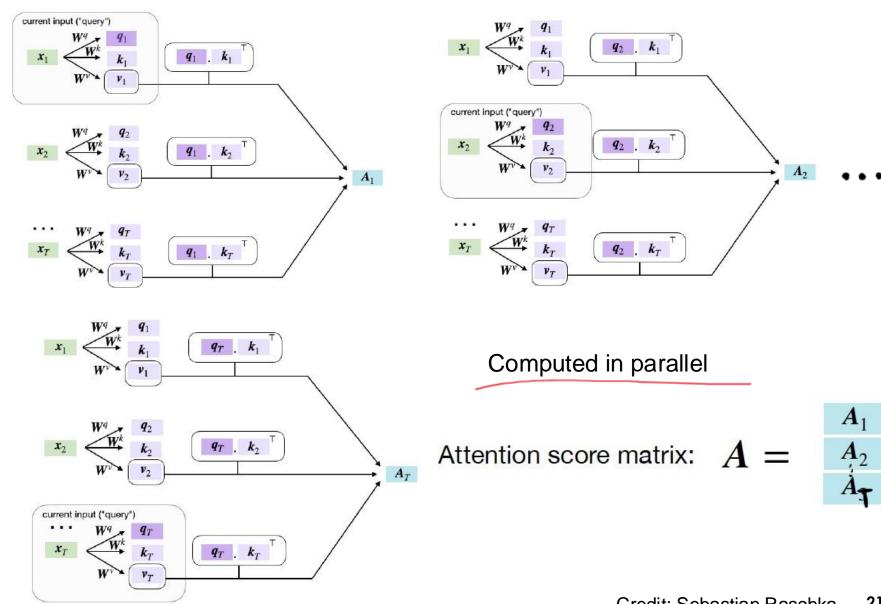




 d_e = embedding size (original transformer = 512) where $d_q = d_k$ $1 \times d_q$ In original transformer, $d_q = d_v$ as well $1 \times d_e$ $1 \times d_{\nu}$ $A(q_2, \mathbf{K}, \mathbf{V}) = \sum_{i=1}^{T} \left[\frac{\exp(q_2 \cdot k_i^{\mathsf{T}})}{\sum_{i} \exp(q_2 \cdot k_i^{\mathsf{T}})} \times \mathbf{v}_i \right]$ current input ("query") A_2 softmax 1×1 $a_{2,T}$ $1 \times d_{\nu}$



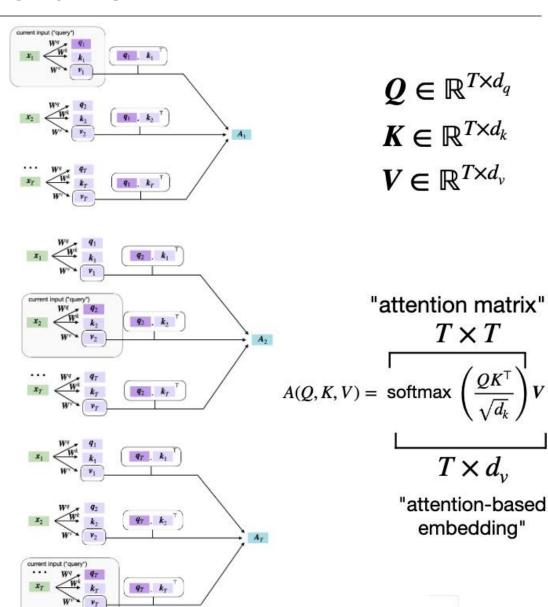
IN COMPUTER VISION



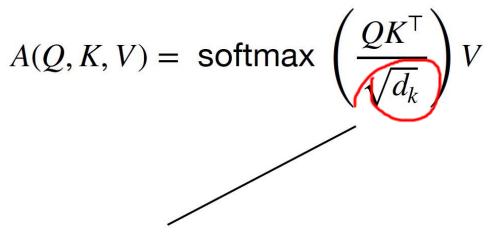
 $d_e = \text{embedding size}$

T = input sequence size



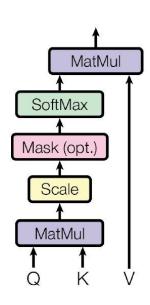


Scaled Dot Product Attention



To ensure that the dot-products between query and and key don't grow too large (and softmax gradient become too small) for large d_k

Scaled Dot-Product Attention



Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

"We suspect that for large values of dk, the dot products grow large in magnitude, pushing the softmax function into regions where it has extremely small gradients."



Summary of self-attention mechanism

Purpose of W_q , W_k , and W_v :

 The input embeddings (or features) of tokens in the sequence are often high-dimensional vectors that encode raw information. However, for attention mechanisms to compute meaningful relationships, these embeddings need to be projected into separate subspaces tailored for the specific roles of query, key, and value.



Summary of self-attention mechanism

W_q (Query projection matrix):

- Projects the input embeddings into the query space.
- This determines how much attention a token will "query" (or ask for) from other tokens.

W_k (Key projection matrix):

- Projects the input embeddings into the key space.
- This determines how the token contributes to the relevance calculation with respect to a query.

W_v (Value projection matrix):

- Projects the input embeddings into the value space.
- This determines what information a token provides when it is attended to.



Summary of self-attention mechanism

Learning Role:

- The weight matrices W_q , W_k , and W_v are learned during the training process through backpropagation. Their purpose is to:
 - Capture and encode different aspects of relationships between tokens in the input sequence.
 - Adapt the model to the specific patterns and dependencies present in the data.
- Having separate weight matrices enhances the ability of the model to encode nuanced relationships between tokens.



- Apply self-attention multiple times in parallel (similar to multiple kernels for channels in CNNs)
- For each head (self-attention layer), use different $\pmb{W}^q, \pmb{W}^k, \pmb{W}^v$, then concatenate the results, $\pmb{A}_{(i)}$
- 8 attention heads in the original transformer, i.e., $W_{(1)}^q, W_{(1)}^k, W_{(1)}^v \dots W_{(8)}^q, W_{(8)}^k, W_{(8)}^v$



Intuition

Capturing Different Types of Relationships:

- Single-head attention may focus on a limited set of features or relationships between tokens because it computes a single attention distribution.
- Multi-head attention allows the model to learn multiple attention distributions simultaneously, each focusing on different aspects of the input sequence.
- For example, one head might focus on long-term dependencies, while another focuses on local context.



Intuition

Learning Diverse Representations:

- Each head has its own set of learnable weight matrices (W_q, W_k, W_v), allowing it to project the input embeddings into different subspaces.
- This enables each head to attend to different features or patterns in the input, leading to a richer and more nuanced representation.



Intuition

Mitigating Information Loss:

- With a single head, compressing all information into one set of attention scores may lose certain details.
- Multi-head attention distributes the representational capacity across multiple attention heads, reducing the risk of losing important information.



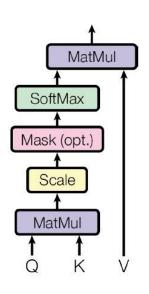
Intuition

Improving Expressiveness:

- By allowing multiple independent attention mechanisms to run in parallel, the model can express a broader range of dependencies and capture more complex interactions in the data.
- For instance, in language modeling, one head might focus on syntactic relationships (e.g., subject-verb agreement), while another focuses on semantic relationships (e.g., thematic roles).



Scaled Dot-Product Attention



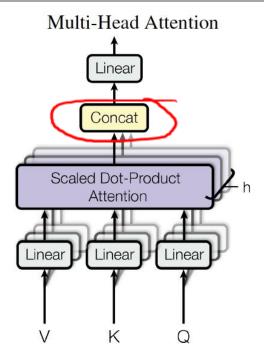
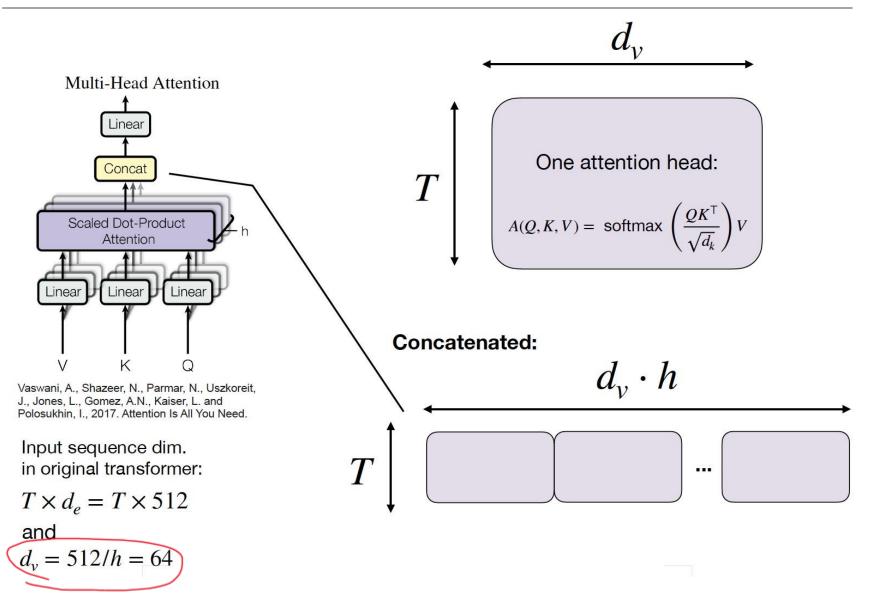


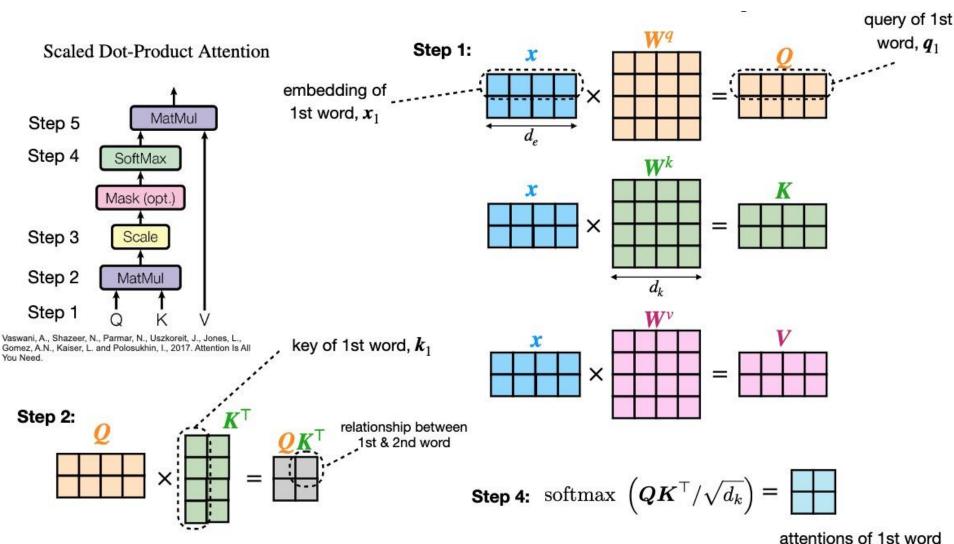
Figure 2: (left) Scaled Dot-Product Attention. (right) Multi-Head Attention consists of several attention layers running in parallel.

$$\begin{split} \text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, ..., \text{head}_{\text{h}}) W^O \\ \text{where } \text{head}_{\text{i}} &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \end{split}$$

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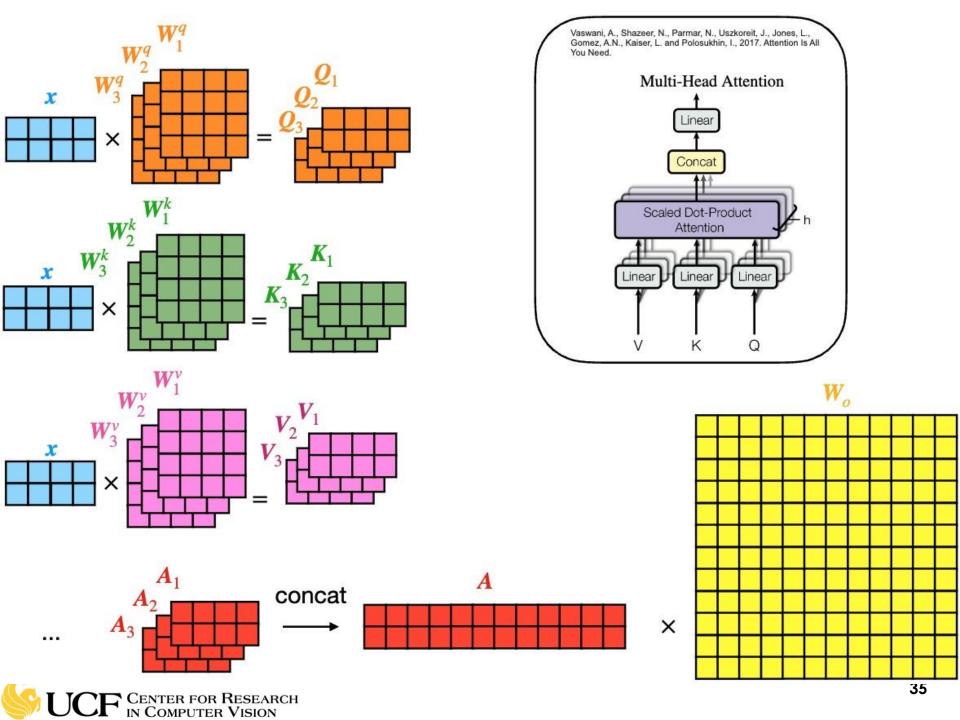


Step 3:

1st value of 1st & 2nd word

with first value of words softmax $\left(QK^{\top}/\sqrt{d_k}\right)$

softmax
$$\left(QK^{\top}/\sqrt{d_k}\right)$$
 V Step 5:



Step-by-Step Walkthrough of Self-Attention in Transformers

1. Input Representation

- Consider an input sequence of n tokens (e.g., words in a sentence).
- Each token is converted into a **word embedding** of size $d_{
 m model} = 512$.
- The input sequence is represented as a matrix:

$$X \in \mathbb{R}^{n imes d_{ ext{model}}}$$

where:

- n = sequence length (e.g., 10 for a short sentence).
- $d_{
 m model} = 512$ (embedding dimension).



2. Linear Projections: Computing Queries, Keys, and Values

Each token embedding is linearly projected into query (Q), key (K), and value (V) vectors using learned weight matrices.

Weight Matrices:

$$W_q \in \mathbb{R}^{d_{ ext{model}} imes d_k}, \quad W_k \in \mathbb{R}^{d_{ ext{model}} imes d_k}, \quad W_v \in \mathbb{R}^{d_{ ext{model}} imes d_v}$$

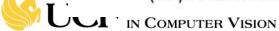
- Typical Dimensions:
 - $d_{
 m model} = 512$ (input embedding size).
 - $d_k=d_q=d_v=64$ (smaller subspace for attention calculations).
 - For multi-head attention: These projections are done separately for each attention head.
- Computing the Projections:

$$Q = XW_a$$
, $K = XW_k$, $V = XW_v$

· The resulting matrices:

$$Q,K,V \in \mathbb{R}^{n imes d_k}$$

(i.e., for a batch of 10 tokens, each of 64-dimensional vectors per head).



3. Compute Scaled Dot-Product Attention

The core self-attention mechanism is computed as:

$$A = rac{QK^T}{\sqrt{d_k}}$$

- Matrix Dimensions:
 - $Q \in \mathbb{R}^{n imes d_k}$ and $K^T \in \mathbb{R}^{d_k imes n}$, so:

$$A = QK^T \in \mathbb{R}^{n imes n}$$

- This forms an attention score matrix where each entry A_{ij} represents how much the ith token attends to the jth token.
- Why Scale by $\sqrt{d_k}$? To prevent large dot product values from dominating the softmax.



4. Apply Softmax to Compute Attention Weights

We apply the **softmax function** along each row of A to normalize attention scores into probabilities:

$$ext{Attention Scores} = ext{softmax} \left(rac{QK^T}{\sqrt{d_k}}
ight)$$

- Dimension after Softmax:
 - $\operatorname{softmax}(A) \in \mathbb{R}^{n \times n}$
 - Ensures each row sums to 1 (probability distribution).



5. Compute Weighted Sum of Values

The final step in attention computation:

$$Output = softmax(A)V$$

- Matrix Multiplication Dimensions:
 - $\operatorname{softmax}(A) \in \mathbb{R}^{n \times n}$
 - $V \in \mathbb{R}^{n \times d_v}$
 - · Resulting attention output:

$$ext{Output} \in \mathbb{R}^{n imes d_v}$$

 This produces an updated representation of each token, contextualized based on attention.



6. Multi-Head Attention

The above steps happen independently for each attention head.

- · Suppose there are 8 heads.
- Each head has its own W_q, W_k, W_v matrices, projecting into $d_k = d_v = 64$ per head.
- Each head processes the input in parallel, producing multiple attention outputs:

$$\operatorname{Head}_i \in \mathbb{R}^{n \times d_k}$$

The outputs of all 8 heads are concatenated:

$$\operatorname{MultiHead}(X) = \operatorname{Concat}(\operatorname{Head}_1, \dots, \operatorname{Head}_8)$$

Final Output Dimension:

$$\mathbb{R}^{n \times (8 \times d_k)} = \mathbb{R}^{n \times 512}$$

- This ensures that the multi-head attention preserves the original embedding size.
- Finally, this concatenated output is projected back to $d_{
 m model}$ using:



7. Feedforward Network (FFN)

 Each token's updated representation from attention is passed through a fully connected feedforward network (FFN):

$$\mathrm{FFN}(X) = \max(0, XW_1 + b_1)W_2 + b_2$$

- Dimensions:
 - $W_1 \in \mathbb{R}^{d_{\mathrm{model}} \times d_{\mathrm{ffn}}}$ with $d_{\mathrm{ffn}} = 2048$.
 - $W_2 \in \mathbb{R}^{d_{\mathrm{ffn}} \times d_{\mathrm{model}}}$.

8. Add & Norm: Residual Connections

Both multi-head attention and FFN have residual connections:

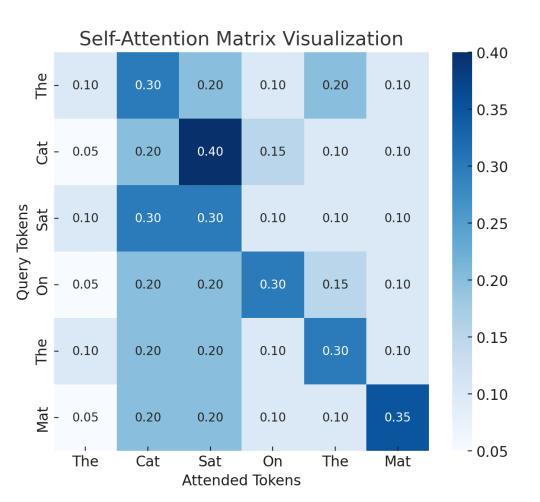
$$X = \operatorname{LayerNorm}(X + \operatorname{MultiHead}(X))$$

$$X = \operatorname{LayerNorm}(X + \operatorname{FFN}(X))$$

These ensure stability and better gradient flow.



Self-attention matrix visualization (an example)

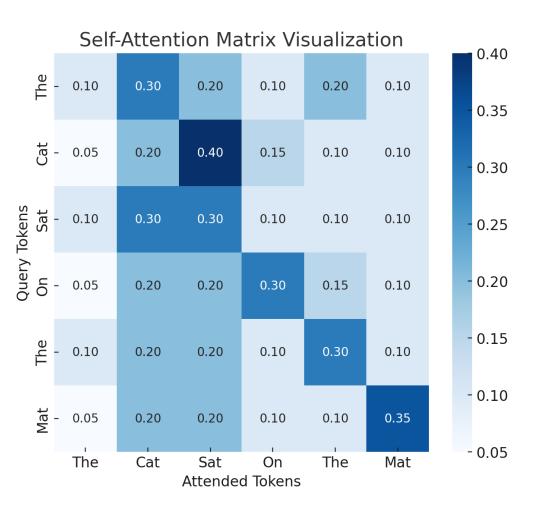


Here is a visual representation of a self-attention matrix for the sentence "The cat sat on the mat."

- Rows: Represent the query tokens (i.e., the token currently attending to others).
- Columns: Represent the tokens being attended to.
- Values (0.0 to 1.0): Represent the attention weight—higher values (darker shades) indicate stronger attention.



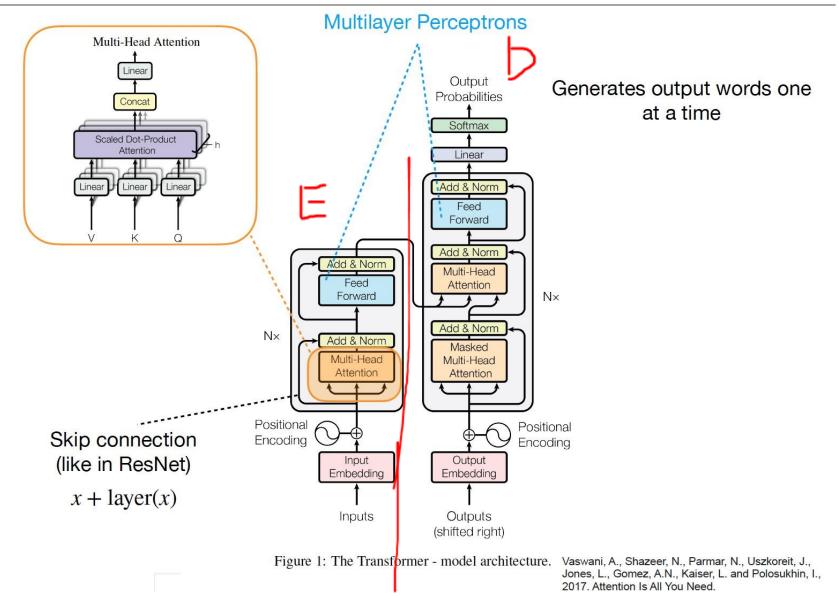
Self-attention matrix visualization (an example)



- The "Cat" row (2nd row) shows high attention to "Sat" (0.4), meaning "Cat" pays the most attention to "Sat."
- The "Mat" row (last row) has a high value (0.35) for itself, meaning it primarily focuses on itself.



The Transformer Architecture





Add Positional Encoding to Word Embedding

 $d_0 = 512$

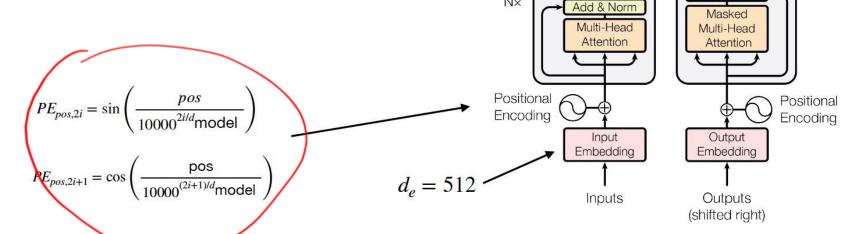
 $N \times$

Add & Norm

Feed

Forward

- Scaled dot-product and fully-connected layer are permutation invariant
- Sinusoidal positional encoding is a vector of small values (constants) added to the embeddings
- As a result, same word will have slightly different embeddings depending on where they occur in the sentence



Position encoding can also be learnable

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L. and Polosukhin, I., 2017. Attention Is All You Need.

Figure 1: The Transformer - model architecture.



Output **Probabilities**

Softmax

Linear

Add & Norm

Feed

Forward

Add & Norm

Multi-Head

Attention

Add & Norm

 $N \times$

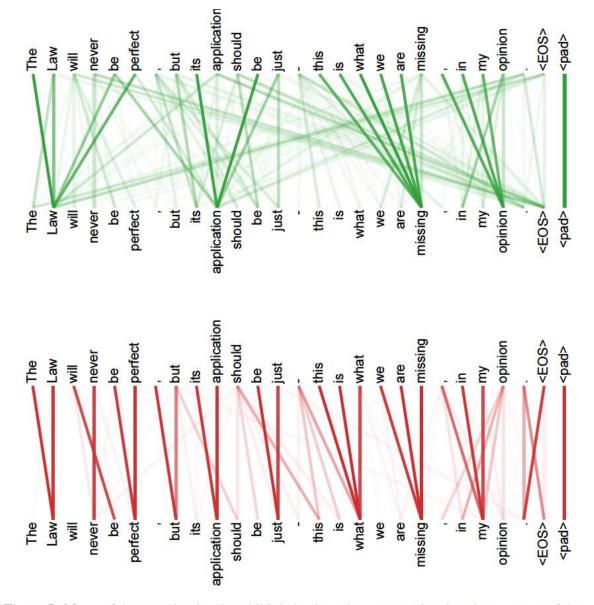


Figure 5: Many of the attention heads exhibit behaviour that seems related to the structure of the sentence. We give two such examples above, from two different heads from the encoder self-attention at layer 5 of 6. The heads clearly learned to perform different tasks.

Attention in transformers, step-by-step
 https://www.youtube.com/watch?v=eMlx5fFNoYc&t=473s



Limitations of Self-Attention Mechanism

Computational Complexity

 The standard attention mechanism computes a similarity matrix between all pairs of tokens, resulting in:

$$\mathcal{O}(n^2 \cdot d)$$

- n: Length of the input sequence.
- d : Embedding dimension.
- This quadratic growth in computation and memory makes it impractical for very long sequences (e.g., documents, long videos, or large medical images).

Memory Bottleneck

- The attention matrix scales with n^2 , which consumes significant GPU/TPU memory, especially for large input sequences or multihead setups.
- This limits batch size and model size during training.



Notable Approaches

(a) FlashAttention

 Key Idea: Memory-efficient attention computation by processing in a chunked, block-wise manner.

Benefits:

- Reduces memory complexity from $\mathcal{O}(n^2)$ to $\mathcal{O}(n \cdot d)$.
- Fused GPU kernels for speed.
- Scalable to long sequences (e.g., tens of thousands of tokens).

Dao, T., Fu, D., Ermon, S., Rudra, A., & Ré, C. (2022). Flashattention: Fast and memory-efficient exact attention with io-awareness. *Advances in Neural Information Processing Systems*, *35*, 16344-16359. Dao, T. (2023). Flashattention-2: Faster attention with better parallelism and work partitioning. *arXiv preprint arXiv:2307.08691*.



Notable Approaches

(b) Sparse Attention

- Key Idea: Leverages the observation that many attention weights are close to zero.
- Only computes attention for a subset of token pairs (sparse patterns like local, random, or strided connections).
- Examples:
 - Longformer: Uses a mix of local and global attention patterns.
 - BigBird: Introduces random, sliding window, and global attention patterns for scalability.
- Complexity: Reduces attention computation to $\mathcal{O}(n \cdot \log n)$ or $\mathcal{O}(n \cdot k)$, where k is the number of non-zero entries.

Beltagy, Iz, Matthew E. Peters, and Arman Cohan. "Longformer: The long-document transformer." *arXiv preprint arXiv:2004.05150* (2020).

Zaheer, Manzil, Guru Guruganesh, Kumar Avinava Dubey, Joshua Ainslie, Chris Alberti, Santiago Ontanon, Philip Pham et al. "Big bird: Transformers for longer sequences." Advances in neural information processing systems 33 (2020): 17283-17297.

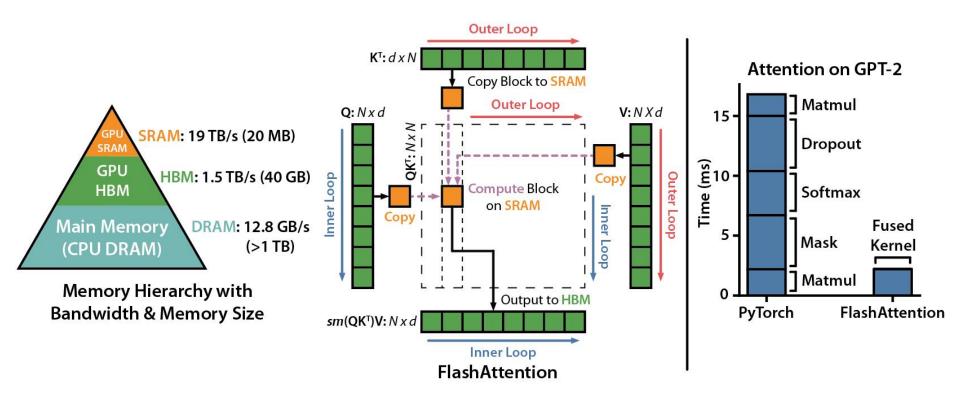


Method	Complexity	Key Feature	Use Case
FlashAttention	$\mathcal{O}(n\cdot d)$	Chunked processing, fused kernels	General-purpose
Longformer	$\mathcal{O}(n\cdot k)$	Local and global attention patterns	Text/document analysis
Linformer	$\mathcal{O}(n\cdot d)$	Low-rank projection of attention	Long text, moderate accuracy
Performer	$\mathcal{O}(n\cdot d)$	Kernelized approximation of softmax	Large-scale tasks
Reformer	$\mathcal{O}(n \cdot \log n)$	LSH-based sparse token grouping	Sparse token interactions

Choromanski, Krzysztof, et al. "Rethinking attention with performers." *arXiv preprint arXiv:2009.14794* (2020). Kitaev, Nikita, Łukasz Kaiser, and Anselm Levskaya. "Reformer: The efficient transformer." *arXiv preprint arXiv:2001.04451* (2020).



FlashAttention



https://github.com/Dao-AlLab/flash-attention

FlashAttention: Fast and Memory-Efficient Exact Attention with IO-Awareness Tri Dao, Daniel Y. Fu, Stefano Ermon, Atri Rudra, Christopher Ré



- Other Approaches
 - Hardware-software co-design (FPGA, etc.)



Vision Transformer (ViT)



AN IMAGE IS WORTH 16x16 WORDS: TRANSFORMERS FOR IMAGE RECOGNITION AT SCALE ____

Alexey Dosovitskiy*,†, Lucas Beyer*, Alexander Kolesnikov*, Dirk Weissenborn*, Xiaohua Zhai*, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, Neil Houlsby*,†

*equal technical contribution, †equal advising
Google Research, Brain Team
{adosovitskiy, neilhoulsby}@google.com

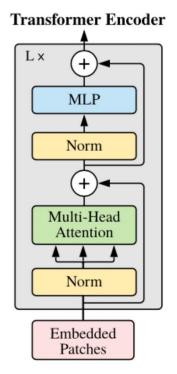
ABSTRACT

While the Transformer architecture has become the de-facto standard for natural language processing tasks, its applications to computer vision remain limited. In vision, attention is either applied in conjunction with convolutional networks, or used to replace certain components of convolutional networks while keeping their overall structure in place. We show that this reliance on CNNs is not necessary and a pure transformer applied directly to sequences of image patches can perform very well on image classification tasks. When pre-trained on large amounts of data and transferred to multiple mid-sized or small image recognition benchmarks (ImageNet, CIFAR-100, VTAB, etc.), Vision Transformer (ViT) attains excellent results compared to state-of-the-art convolutional networks while requiring substantially fewer computational resources to train.¹

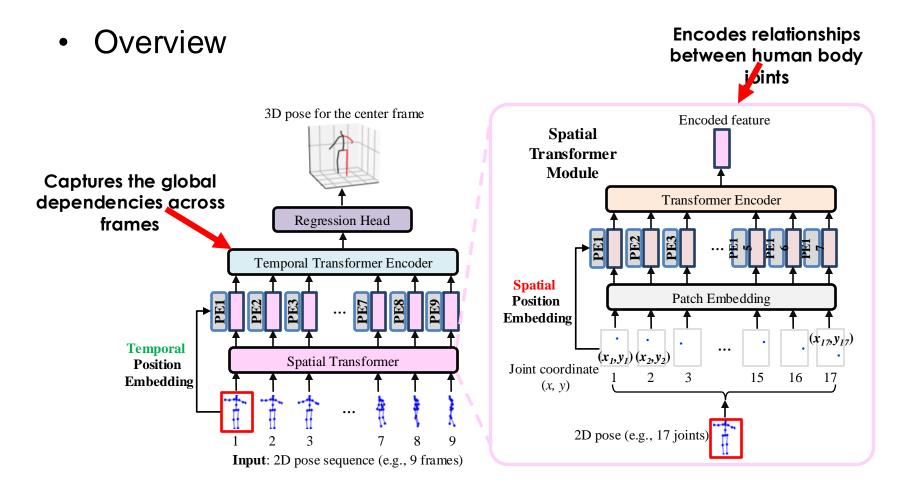


Vision Transformer





Other applications (ViT for Human Pose Estimation)

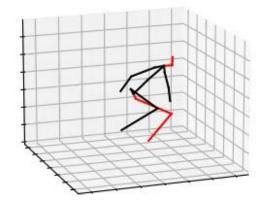




Zheng, Ce, et al. "3d human pose estimation with spatial and temporal transformers." Proceedings of the IEEE/CVF International Conference on Computer Vision. 2021.

Video with heavy occlusion









What is Cross-Attention

1. Self-Attention vs. Cross-Attention

- Self-Attention: The query (Q), key (K), and value (V) all come from the same input (e.g., a sentence in NLP or patches in ViTs).
- Cross-Attention: The query (Q) comes from one modality (e.g., text) while the keys (K) and values (V) come from another modality (e.g., image features).

2. Cross-Attention in Multi-Modal Models

- Used in models that integrate multiple input types, such as:
 - Vision-Language Models (e.g., CLIP, Flamingo) → Image ↔ Text
 - Video Question Answering → Video Frames ↔ Text Question
 - Speech-Text Models (e.g., Whisper) → Audio ↔ Text



What is Cross-Attention

3. Cross-Attention Computation

$$A = \operatorname{softmax}\left(rac{Q_T K_I^T}{\sqrt{d_k}}
ight)$$

 $\operatorname{CrossAttention} \operatorname{Output} = AV_I$

- Q_T (Queries) → From Text Tokens
- K_I, V_I (Keys, Values) → From Image Features (e.g., CNN/Vision Transformer)
- Softmax ensures the text tokens attend to relevant image features.



Example - Image Captioning using Cross-Attention

Use Case: Generating Captions for an Image

- Input:
 - Image → Processed via CNN/ViT → Produces image embeddings.
 - Text (e.g., partial caption) → Used to generate queries (Q).

Cross-Attention:

- The text queries attend to image features to determine the most relevant visual information.
- Used in image captioning models like BLIP and Flamingo.



Resources

Surveys

- Transformers in Vision: A Survey https://arxiv.org/abs/2101.01169
- A Survey on Vision Transformer https://arxiv.org/abs/2012.12556
- Transformers in Medical Imaging: A Survey https://arxiv.org/pdf/2201.09873.pdf
- Efficient Transformers: A Survey https://arxiv.org/pdf/2009.06732.pdf

the memory and computational complexity required to compute the attention matrix is quadratic in the input sequence length

Codes

- https://huggingface.co/docs/transformers/index
- https://github.com/dk-liang/Awesome-Visual-Transformer
- https://github.com/fahadshamshad/awesome-transformers-in-medicalimaging



Thank you!

Question?

