Transformers

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Motivation for Transformers

- **Limited Context:**
  - RNNs process sequences step-by-step $\rightarrow$ Difficult to capture long-range dependencies.
  - CNNs are effective for local patterns $\rightarrow$ Struggle with global context in sequences.
- **Sequential Bottlenecks:**
  - RNNs process data sequentially.
  - Prevents efficient parallelization.
  - Leads to slow training and inference.
- **Slow Training:**
  - RNNs and CNNs are computationally intensive.
  - Especially challenging for long sequences or large images.
  - Results in increased training times.

Motivation for Transformers (cont.)

There is a need for models that:

- Capture comprehensive, global context efficiently.
- Allow for parallel computation.
- Accelerate training and inference.

Transformers address these needs by:

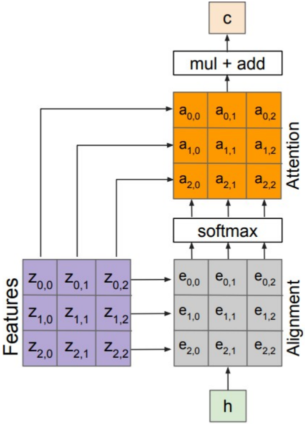
- Leveraging self-attention mechanisms.
- Modeling dependencies across entire sequences.
- Enabling highly parallelizable computation.

Learning Outcomes

After this lecture, you will be able to:

- Explain the motivation behind the development of Transformers.
- Describe the architecture and key components of Transformer models.
- Understand and implement attention and self-attention mechanisms.
- Explain the role of positional encoding in Transformers.
- Distinguish between general attention and self-attention.
- Understand the concept and benefits of multi-head attention.
- Compare CNNs with and without self-attention.
- Summarize the advantages of Transformers over traditional sequence models.

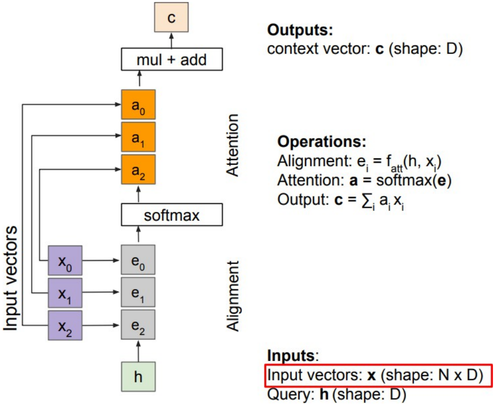
- Previously, we saw how attention helps image captioning models focus on important regions, generating more relevant captions.
- However, we noticed limitations—attention sometimes misses subtle details or struggles with complex scenes.



Outputs:
context vector: **c** (shape: D)

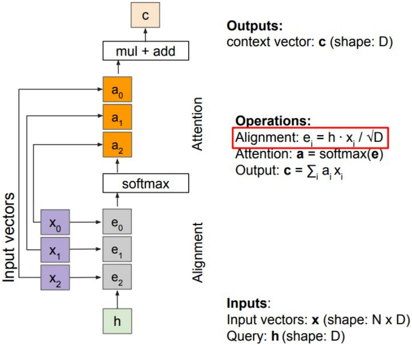
Operations:
Alignment: $e_{i,j} = f_{att}(h, z_{i,j})$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $\mathbf{c} = \sum_{i,j} a_{i,j} z_{i,j}$

Inputs:
Features: **z** (shape: H x W x D)
Query: **h** (shape: D)



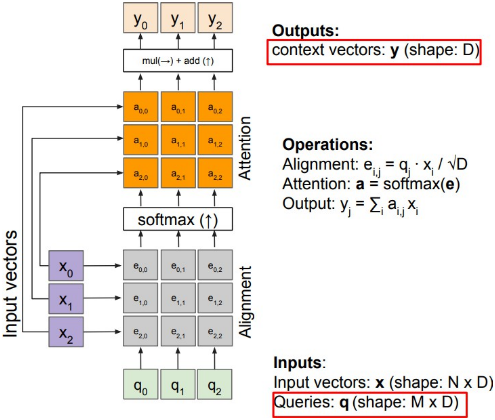
- The **attention** operation is permutation invariant.
- It does not depend on the ordering of features.
- Reshape the input of size $H \times W = N$ into N feature vectors.

General Attention Layer (cont.)



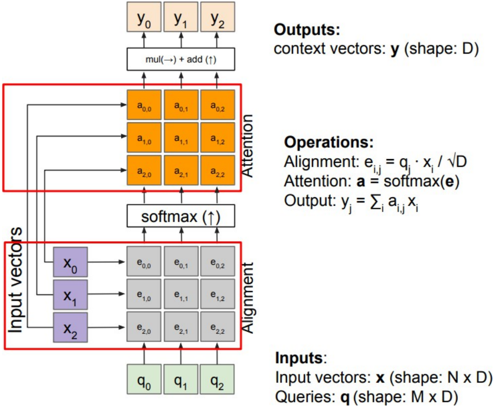
- The original attention mechanism $f_{att}(.)$ uses a simple dot product to compute similarity between queries and keys.
- As the feature dimension D increases $\rightarrow$ the dot product sum involves more terms $\rightarrow$ larger variance in the resulting logits.
- Larger magnitude vectors produce higher logits $\rightarrow$ causing the softmax output to become more peaked (lower entropy, assuming logits are IID).
- This means the **model may focus too narrowly**, assigning very **high attention to a few positions** and **almost none to others**.
- To counteract this $\rightarrow$ we scale the dot product by dividing by $\sqrt{D}$.
- This normalization keeps the variance of the logits more consistent, resulting in a softer, more balanced attention distribution.

General Attention Layer (cont.)



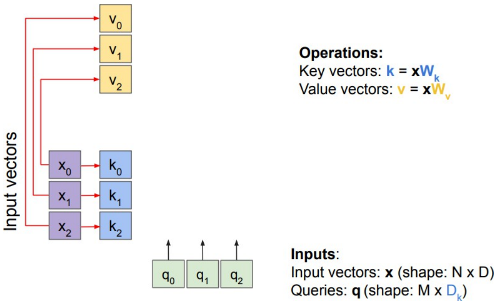
- We can use multiple **query vectors** in the attention mechanism.
- Each query attends to the input independently, producing its own output context vector.
- This allows the model to extract different types of information from the same input, enabling richer and more flexible representations.

General Attention Layer (cont.)

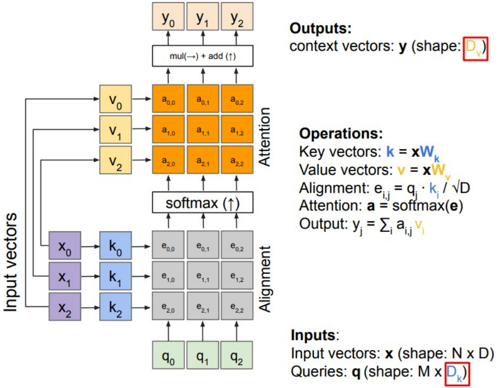


- Observe that the same input vectors are used for both computing the alignment scores (queries and keys) and for generating the attention-weighted output (values).
- This dual use lets the model efficiently use the same features for both attending and aggregating information.

General Attention Layer (cont.)

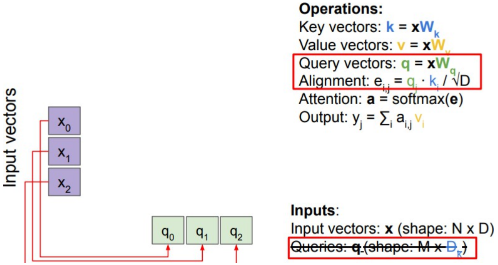


- Notice that the same input vectors are used for both computing alignment scores (as queries and keys) and for generating the attention-weighted output (as values).
- To increase the expressiveness of the attention layer, we can introduce separate fully connected (FC) layers before each step → one for queries, one for keys, and one for values.
- This allows the model to learn different transformations for each role, enabling richer and more flexible representations.



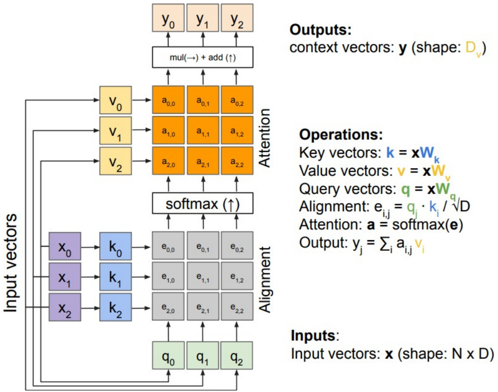
- The input vectors are used for both computing alignment scores (as queries and keys) and for generating the attention-weighted output (as values).
- To enhance the expressiveness of the attention layer, we introduce separate fully connected (FC) layers for queries, keys, and values.
- Each FC layer can learn a different transformation, allowing the model to capture more complex relationships.
- With this setup, the input and output dimensions can differ, depending on the transformations applied by the key and value FC layers.

Self Attention Layer



- Recall: the query vector is derived from the input vectors.
- In a self-attention layer, query, key, and value vectors are all computed from the same input.
- There are no separate input query vectors; instead, they are generated internally.
- Typically, fully connected (FC) layers are used to compute the query, key, and value vectors from the input.
- This allows each position in the input to attend to all other positions, enabling the model to capture contextual relationships.

Self Attention Layer (cont.)



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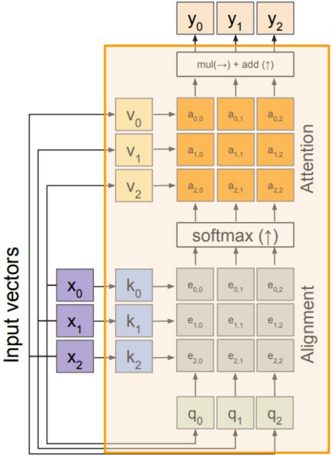
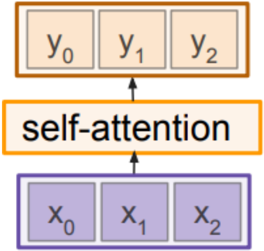
Self Attention Layer (cont.)



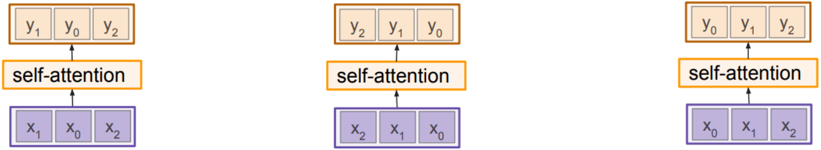
Outputs:
context vectors: **y** (shape: D_v)

Operations:
Key vectors: $\mathbf{k} = \mathbf{x}W_k$
Value vectors: $\mathbf{v} = \mathbf{x}W_v$
Query vectors: $\mathbf{q} = \mathbf{x}W_q$
Alignment: $e_{i,j} = q_j \cdot k_i / \sqrt{D}$
Attention: $\mathbf{a} = \text{softmax}(\mathbf{e})$
Output: $y_j = \sum_i a_{i,j} v_i$

Inputs:
Input vectors: **x** (shape: N x D)



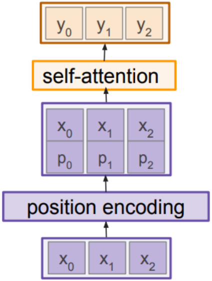
Permutation Invariance



- The self-attention layer is **permutation equivariant**: it produces the same output regardless of the order of the input elements.
- This means the model does not inherently capture the order of the sequence.
- **Challenge:** For tasks involving ordered data, such as language or images, we need a way to encode positional information.
- *How can we enable the model to distinguish between different positions in a sequence?*

Permutation Invariance

- **Positional Encoding:** Supplies sequence order information to models that lack recurrence or convolution, such as Transformers.
- Concatenate or add a special positional encoding p_j to each input vector x_j.
- A function $\mathrm{pos} : \mathbb{N} \to \mathbb{R}^D$ maps the position j of the vector into a D-dimensional vector, i.e., $p_j = \mathrm{pos}(j)$.



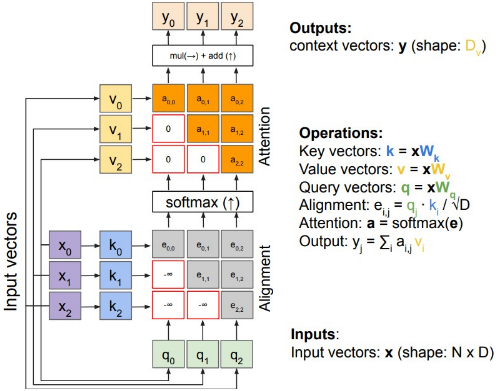
Permutation Invariance (cont.)

- The positional encoding is added to the input vectors before computing the attention scores.
- This allows the model to incorporate information about the position of each vector in the sequence.
- The positional encoding can be learned or fixed, depending on the implementation.
- The choice of positional encoding can affect the model's ability to capture long-range dependencies and relationships in the data.
- **Sinusoidal encodings:** Common fixed positional encoding uses sine and cosine functions:

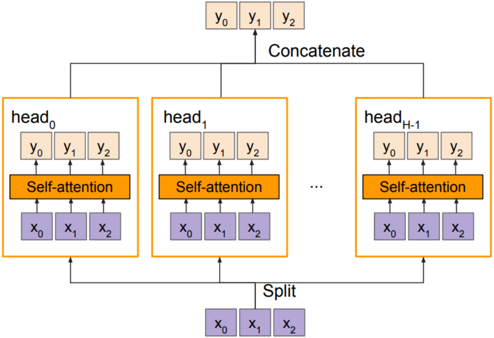
$$\mathrm{pos}(j)_{2k} = \sin\left(\frac{j}{10000^{2k/d}}\right)$$

$$\mathrm{pos}(j)_{2k+1} = \cos\left(\frac{j}{10000^{2k/d}}\right)$$

Masked Self-Attention Layer

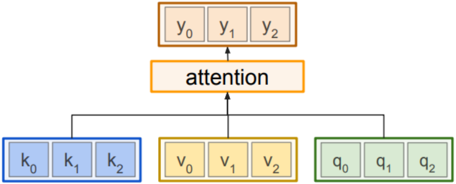


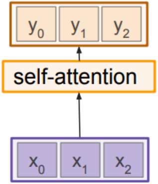
- Prevents each position from attending to subsequent (future) positions.
- Achieved by setting (manually) alignment scores of future tokens to $-\infty$ before softmax.
- Ensures predictions for position i depend only on positions $\leq i$.



- Instead of a single attention mechanism, use multiple “heads” operating in parallel.
- Each head attends to different parts or aspects of the input, capturing diverse relationships (e.g., subject-verb, coreferences).
- The outputs from all heads are concatenated and projected, resulting in a richer and more expressive context representation.
- This modular approach allows the model to learn various types of dependencies simultaneously, improving overall performance.

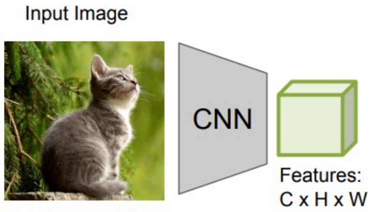
General-Attention Vs Self-Attention





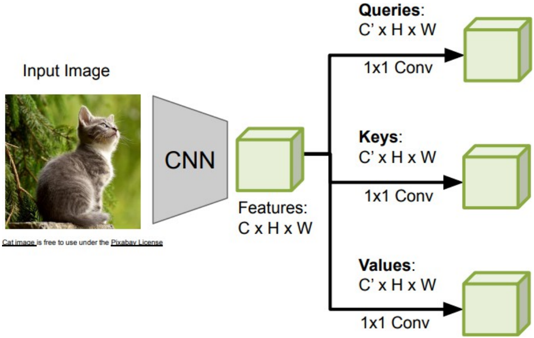
Comparison	**General Attention**	**Self-Attention**
Q, K, V origins	From separate source & target	From same input sequence
Use case	Encoder $\rightarrow$ Decoder cross-attention	Encoder/Decoder internal relation info
Information flow	Across representations	Within single representation

Table 1: General Attention vs. Self-Attention

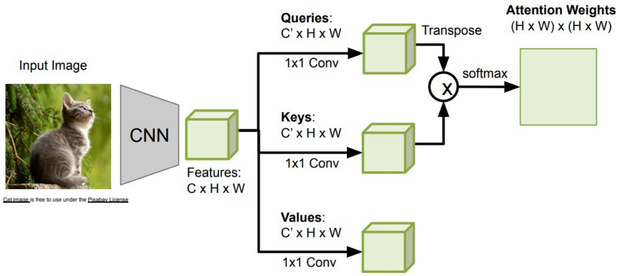


Input Image
CNN
Features:
C x H x W

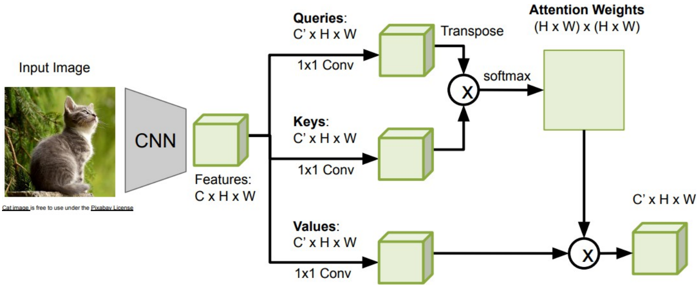
Example: CNN with Self-Attention (cont.)



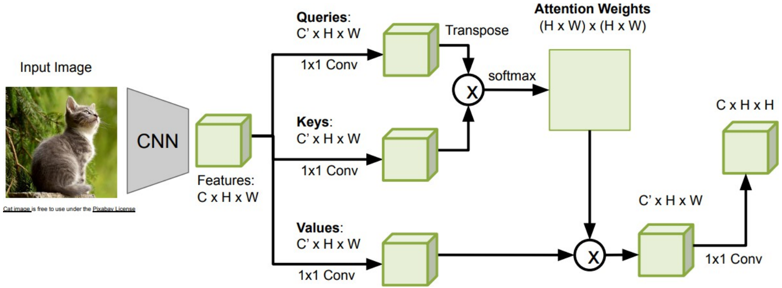
Example: CNN with Self-Attention (cont.)



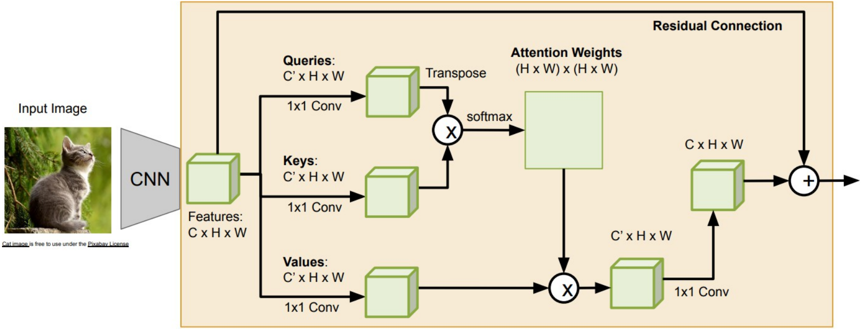
Example: CNN with Self-Attention (cont.)



Cat image is free to use under the Pixabay License


Input Image
CNN
Features:
C x H x W
Queries:
C' x H x W
1x1 Conv
Keys:
C' x H x W
1x1 Conv
Values:
C' x H x W
1x1 Conv
Transpose
softmax
Attention Weights
(H x W) x (H x W)
x
x
C' x H x W
1x1 Conv
C x H x H
Cat image is free to use under the Pixabay License

Example: CNN with Self-Attention (cont.)



Self-Attention Module

Attention is all you need

Vaswani et al, NeurIPS 2017

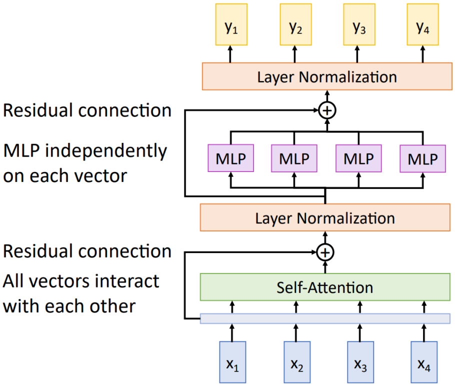


Figure 2: Detailed view of a single Transformer block.

- **Input:** A set of vectors **x**, one per token.
- **Output:** A set of vectors **y**, one per token.
- **Self-Attention:** Allows each token to attend to all others, capturing contextual relationships.
- **Layer Normalization & MLP:** Applied independently to each token, ensuring stability and expressiveness.
- **Key Properties:** Highly scalable and parallelizable due to independent operations across tokens.

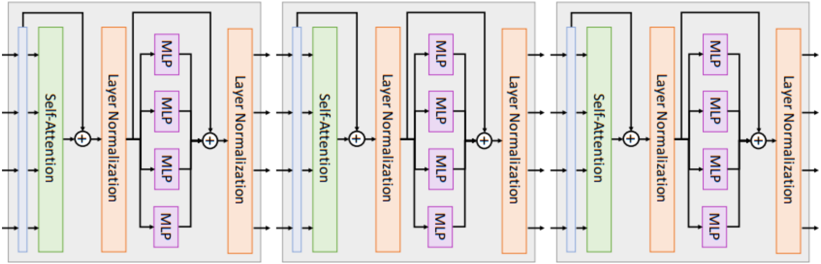


Figure 3: Stacking multiple Transformer blocks.

- A Transformer consists of a sequence of identical blocks, each refining the token representations.
- In the original architecture (Vaswani et al., 2017): 12 blocks, hidden size $D_Q = 512$, and 6 attention heads were used.
- The modular design enables deep stacking and efficient parallel computation.

Summary

- Transformers use self-attention to capture relationships within sequences.
- Self-attention allows each token to attend to all other tokens, enabling context-aware representations.
- Positional encoding is crucial for maintaining the order of tokens in the sequence.
- Masked self-attention prevents future information leakage during training.
- Multi-head attention enhances model capacity by allowing multiple attention mechanisms to learn different aspects of the data.

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Credits

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This project benefited from external collaboration, and we acknowledge their contribution with gratitude.