Unveiling the Power of Attention: A Deep Dive into Attention Mechanisms

Bilal FAYE, Nicolas FLOQUET

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Introduction To Attention Mechanism

An attention mechanism in the context of machine learning refers to a computational model that allows a system to selectively focus on certain parts of input data while ignoring others.

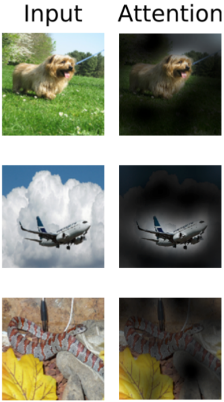


Figure – Attention Visualization on Image Classification [1]

1. Dosovitskiy et al., An Image is Worth 16x16 Words : Transformers for Image Recognition, 2020

Some key points highlighting the powerful aspects of attention mechanisms :

- Resource Allocation Efficiency
- Wide Range Applications
- Interpretable Neural Architectures
- Enhanced Performance in Specific Tasks
- Intuitive Explanations for Neural Behaviors

Broad Understanding of Attention Mechanisms

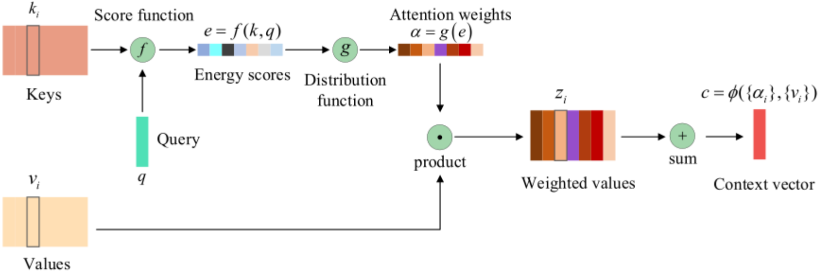


Figure – Unified Attention Model [2]

2. Zhaoyang et al., A review on the attention mechanism of deep learning, 2021

- **Keys** : This refers to the input data representations on which the model relies to identify relevant information or patterns in the sequence.

- **Query** : This represents what the model aims to search for or extract from the input data.

- **Values** : This corresponds to the actual information associated with each part of the input data (sequence).

The score function $\mathbf{e} = \mathbf{f}(\mathbf{k}, \mathbf{q})$ determines the matching or combination of keys and queries.

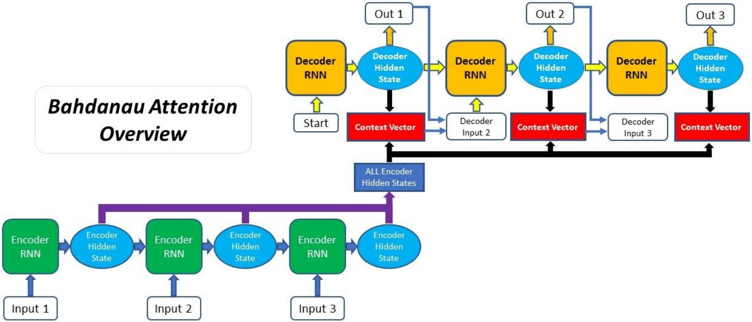
Additive attention [3] combines keys and queries through a summation operation :

Additive score function

$$\mathbf{f}(\mathbf{q}, \mathbf{k}) = \mathbf{v}^{\mathbf{T}}\mathbf{activation}(\mathbf{W_1 k} + \mathbf{W_2 q})$$

where $\mathbf{v}$, $\mathbf{W_1}$ and $\mathbf{W_2}$ are learnable parameters.

3. Bahdanau et al., Neural Machine Translation by Jointly Learning to Align and Translate, 2014


Bahdanau Attention Overview
Out 1
Out 2
Out 3
Decoder RNN
Decoder Hidden State
Decoder RNN
Decoder Hidden State
Decoder RNN
Decoder Hidden State
Start
Context Vector
Decoder Input 2
Context Vector
Decoder Input 3
Context Vector
ALL Encoder Hidden States
Encoder RNN
Encoder Hidden State
Encoder RNN
Encoder Hidden State
Encoder RNN
Encoder Hidden State
Input 1
Input 2
Input 3

Broad Understanding of Attention Mechanisms

Multiplicative (dot-product) attention [4] computes the relevance between keys and queries by taking their dot product :

Multiplicative score function

$$\mathbf{f}(\mathbf{q}, \mathbf{k}) = \mathbf{q}^{\mathbf{T}}\mathbf{k}$$

In WMT'15 English → German task [5], authors found that parameterized additive attention slightly outperformed multiplicative attention.

4. Luong et al., Effective Approaches to Attention-based Neural Machine Translation, 2015
5. Britz et al., Massive exploration of neural machine translation architectures, 2017

Broad Understanding of Attention Mechanisms

Scaled multiplicative (dot-product) attention [6] computes the relevance between keys and queries by taking their dot product :

Scaled multiplicative score function

$$\mathbf{f}(\mathbf{q}, \mathbf{k}) = \frac{\mathbf{q}^{\mathbf{T}}\mathbf{k}}{\sqrt{\mathbf{d_k}}}$$

where $\mathbf{d_k}$ is the dimension of keys.

For small values of $\mathbf{d_k}$, both mechanisms perform similarly, but additive attention outperforms multiplicative attention without scaling for larger $\mathbf{d_k}$.

6. Vaswani et al., Attnetion is all you need, 2017

General attention [7] extends the concept of multiplicative attention by introducing a learnable matrix parameter $\mathbf{W}$:

General score function

$$\mathbf{f(q, k) = q^T W k}$$

where $\mathbf{W}$ is a learnable parameter.

This approach is applicable to keys and queries with distinct representations.

7. Luong et al., Effective Approaches to Attention-based Neural Machine Translation, 2015

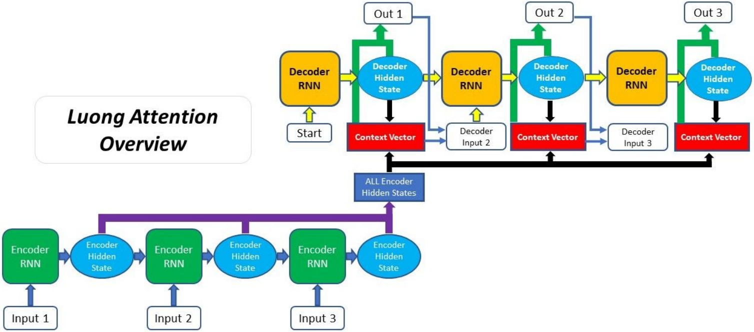
Concat attention [8] aims to derive the joint representation of the keys and queries instead of comparing them :

Concat score function

$$\mathbf{f}(\mathbf{q}, \mathbf{k}) = \mathbf{v}^{\mathbf{T}}\mathbf{activation}(\mathbf{W}[\mathbf{k}; \mathbf{q}])$$

where **W** is a learnable parameter.

8. Luong et al., Effective Approaches to Attention-based Neural Machine Translation, 2015


Luong Attention Overview
Out 1
Out 2
Out 3
Decoder RNN
Decoder Hidden State
Decoder RNN
Decoder Hidden State
Decoder RNN
Decoder Hidden State
Start
Context Vector
Decoder Input 2
Context Vector
Decoder Input 3
Context Vector
ALL Encoder Hidden States
Encoder RNN
Encoder Hidden State
Encoder RNN
Encoder Hidden State
Encoder RNN
Encoder Hidden State
Input 1
Input 2
Input 3

Location-based attention [9] are solely computed from the target hidden state :

Location-based score function

$$\mathbf{f}(\mathbf{q}, \mathbf{k}) = \mathbf{f}(\mathbf{q})$$

Energy scores ($\mathbf{f}$) depend solely on $\mathbf{q}$ rather than $\mathbf{K}$. Conversely, self-attention is calculated solely based on $\mathbf{K}$, without requiring $\mathbf{q}$.

9. Luong et al., Effective Approaches to Attention-based Neural Machine Translation, 2015

Similarity attention [10] compares the similarity between $\mathbf{K}$ and $\mathbf{q}$, which relied on cosine similarity. :

Similarity score function

$$\mathbf{f}(\mathbf{q},\mathbf{k}) = \frac{\mathbf{q}\cdot\mathbf{k}}{\|\mathbf{q}\|\cdot\|\mathbf{k}\|}$$

Similarity attention is crucial in :

- semantic similarity assessments (in NLP)
- feature-based comparisons (in CV)

10. Graves et al., Neural turing machines, 2014

The distribution function **g** corresponds to the softmax, logistic or sigmoid, which normalize all the energy scores to a probability distribution.

After calculating attention weights and values, the context vector c is computed as follows :

Context vector

$$\mathbf{c} = \phi(\{\alpha_{\mathbf{i}}\}, \{\mathbf{v_i}\}),$$

where ϕ is a function that returns a single vector given the set of values and their corresponding weights.

$$\mathbf{z_i} = \alpha_{\mathbf{i}} \mathbf{v_i},$$

and

$$\mathbf{c} = \sum_{\mathbf{i=1}}^{\mathbf{n}} \mathbf{z_i},$$

where $\mathbf{z_i}$ is a weighted representation of an element in values and n is the dimension of $\mathbf{Z}$.

Categories of Attention Mechanisms

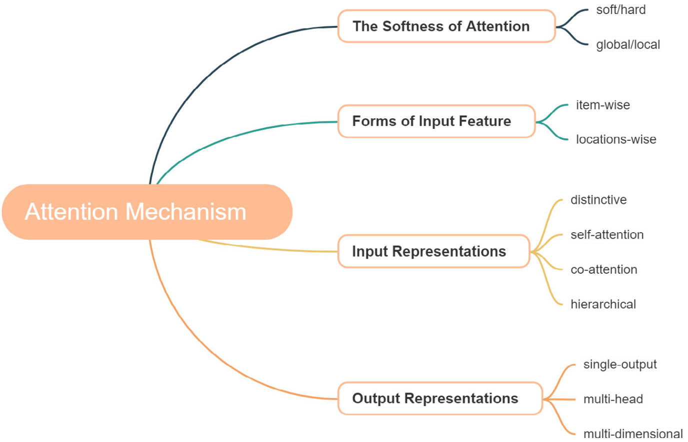


Figure – Unified Attention Model [11]

11. Zhaoyang et al., A review on the attention mechanism of deep learning, 2021

Categorie 1 : The Softness of Attention

- **Soft Attention :**
  - **Definition :** Soft (deterministic) attention calculates a context vector through a weighted average of all keys, facilitating differentiability with respect to inputs, thus enabling training via standard backpropagation methods.

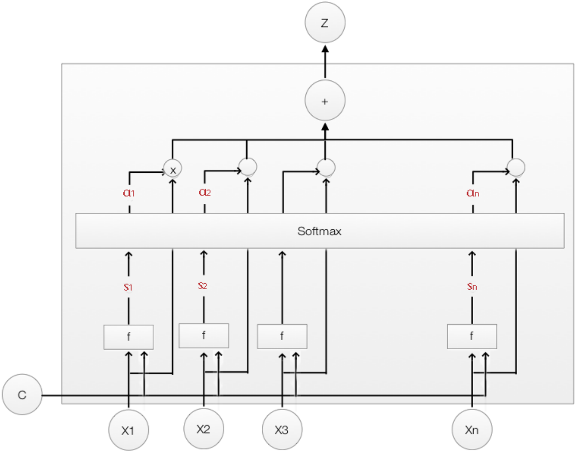


Figure – An instance demonstrating the application of soft attention.

- **Hard Attention :**
  - **Definition :** Hard (stochastic) attention is an attention mechanism that makes discrete decisions regarding which parts of the input sequence to focus on, resulting in non-differentiability with respect to inputs, thereby complicating training using standard backpropagation methods.

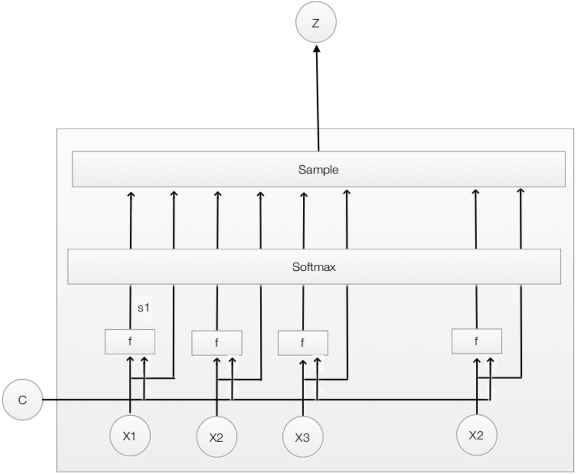
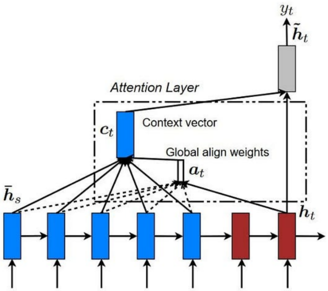
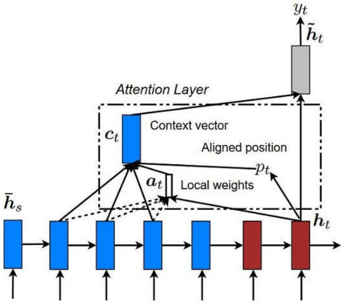


Figure – An instance demonstrating the application of hard attention.

- **Global Attention :**
  - **Definition :** Global attention is similar to soft attention, all source words are considered at a time.



- **Local Attention :**
  - **Definition :** In Local attention, only a subset of source words are considered at a time.



Categorie 2 : Form of Input Feature

- **Item-wise attention**
  - **Definition :** The item-wise attention requires that the input is either explicit items or an additional preprocessing (ex. word embeddings) step is added to generate a sequence of items (vectors) from the source data.
  - item-wise soft attention calculates a weight for each item, and then makes a linear combination of them.
  - Instead of a linear combination of all items, the item-wise hard attention stochastically picks one or some items based on their probabilities.

- **Location-wise attention**
  - **Definition :** location-wise attention is aimed at tasks that are difficult to obtain distinct input items (visual tasks).
  - The location-wise soft attention accepts an entire feature map as input and generates a transformed version through the attention module.
  - The location-wise hard attention stochastically picks a sub-region as input and the location of the sub-region to be picked is calculated by the attention module.

Categorie 3 : Input Representations

- **Distinctive Attention :**
  - **Definition :** Distinctive attention, as defined in the mentioned context, involves attention models with a single input and corresponding output sequence, where keys and queries are derived from two independent sequences.

- **Self-Attention :**
  - **Definition :** Self-attention is an attention mechanism in which each element in a sequence attends to all other elements in the same sequence.

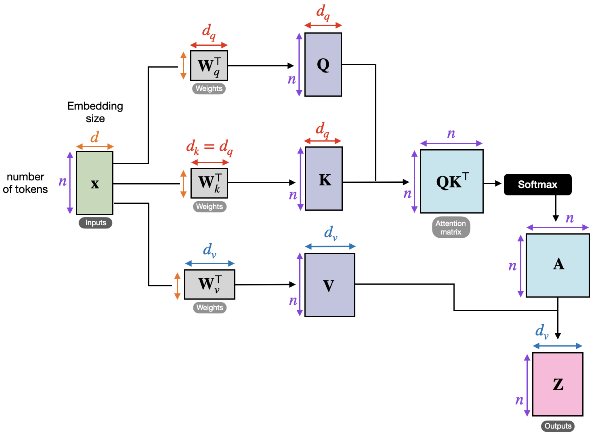


Figure – Application of self-attention

- **Cross-Attention :**
  - **Definition :** Cross-attention refers to scenarios where attention is applied between different parts of the input and output sequences.

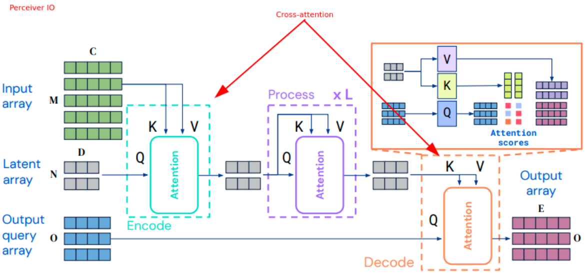


Figure – Application of cross-attention

- **Co-Attention :**
  - **Definition :** Co-attention refers to an attention mechanism that simultaneously considers and aligns information from multiple input sequences or modalities. co-attention can be coarse-grained [12] or fine-grained [13].

12. Coarse-grained attention computes attention on each input, using an embedding of the other input as a query

13. Fine-grained attention evaluates how each element of an input affects each element of the other input

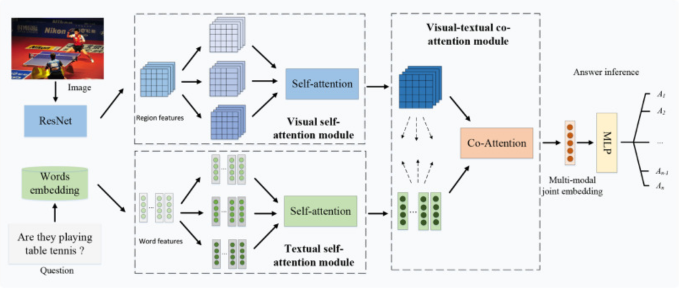


Figure – Application of co-attention

- **Hierarchical Attention :**
  - **Definition :** Hierarchical attention allows the computation of attention weights not only from the original input sequence but also from different abstraction levels (ex. document classification).

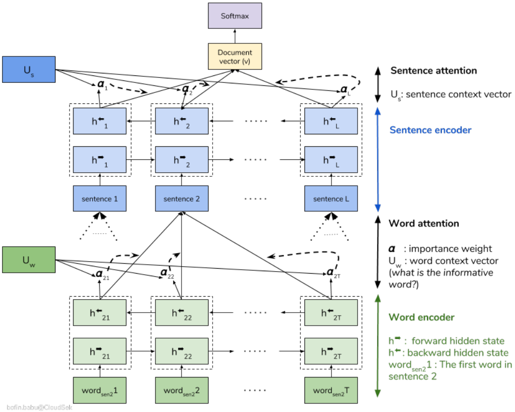


Figure – Application of hierarchical attention

Categorie 4 : Output Representations

- **Single Output Attention :**
  - **Definition :** The energy scores are represented by one and only one vector at each time step.

- **Multi-Head Attention :**
  - **Definition :** An attention mechanism that employs multiple attention heads to capture diverse features and relationships in parallel.

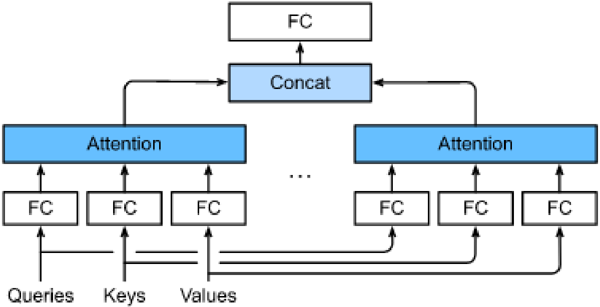


Figure – Application of multi-head attention

- **Multi-Dimensional Attention :**
  - **Definition :** An approach that computes a feature-wise score vector for keys by replacing weight scores vector with a matrix. In this way, the neural network can calculate multiple attention distributions for the same data.

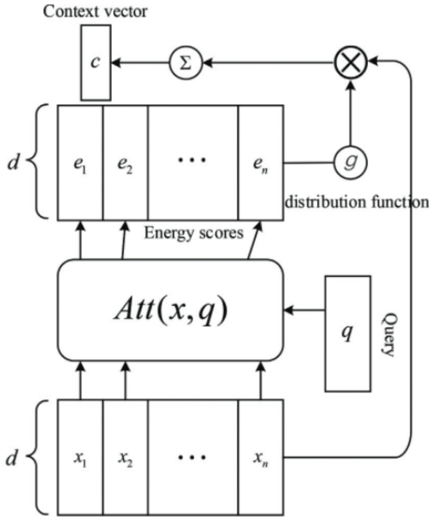


Figure – Application of multi-dimensional attention