Transformer Tutorial

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Ming Li, CS 886, Waterloo University
Jay Alammar, "The Illustrated Transformer"
Xipeng Qiu, "*A Tutorial of Transformers", Fudan University*
Aman Arora, https://amaarora.github.io/2021/01/18/ViT.html

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Overview

- Attention
- Transformer Introduction
- Self-attention and Multi-head self-attention
- Position Encoding
- Residual and Decoder
- Transformer Variants in NLP
- Vision Transformer
- Codes for Vision Transformer
- Recent Vision Transformer Paper

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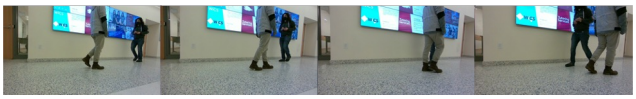
Overview

- Transformers were created for processing *sequential data*:
  - Natural language (sequence of words):

She ate a green apple

  - Video (sequence of images):



  - Output can be another sequence

She ate a green apple → **Elle a mangé une pomme verte**

English French

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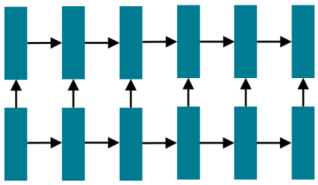
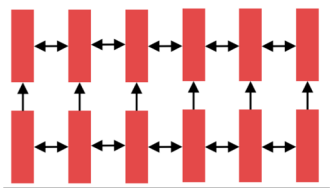
Models for sequential data are not new

- Recurrent models:
  - Recurrent Neural Networks (RNNs)
    - Long Short-Term Memory Networks (LSTMs)
      - Bi-directional LSTMS ....





- Why are these methods surpassed by Transformer?

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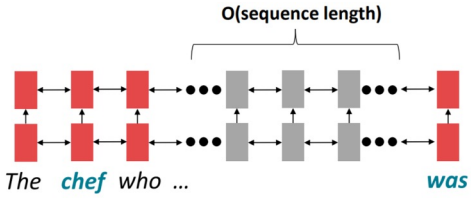
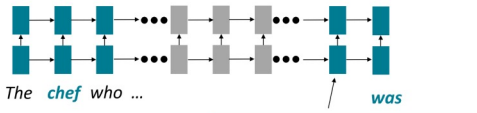
Recurrent Models have long interaction distance

- Taking O(sequence length) steps for distant units to interact



- Meaning that hard to long-distance relations
  - Both Information and gradient flow through so many layers



Info of ***chef*** has gone through O(sequence length) many layers!

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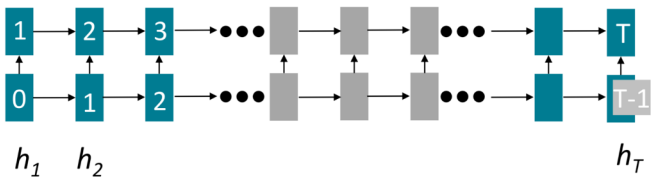
Recurrent Models lack parallelizability

- Forward and backward passes have O(sequence length)
  - Later states are computed only after previous states are computed
  - Hard to train on long sequences, large datasets
- GPU is not good at this "serial" computation
  - Instead, it can do many independent computations in parallel



Numbers indicate min # of steps before a state can be computed

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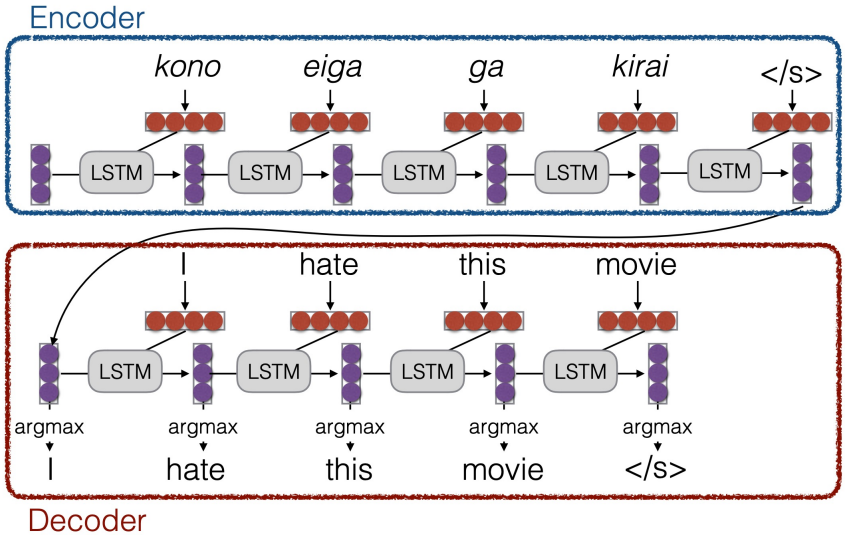
Encoder-Decoder Models



Sutskever et al. "Sequence to sequence learning with neural networks", NeurIPS 2014

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Problem of Sentence Representation:

"You can't cram the meaning of a whole %&!$ing sentence into a single $&!*ing vector!" — Ray Mooney

Basic idea of Attention:

- Encode each word in the sentence into a vector
- When decoding, perform a linear combination of these vectors, weighted by "attention weights"
- Use this combination in picking the next word

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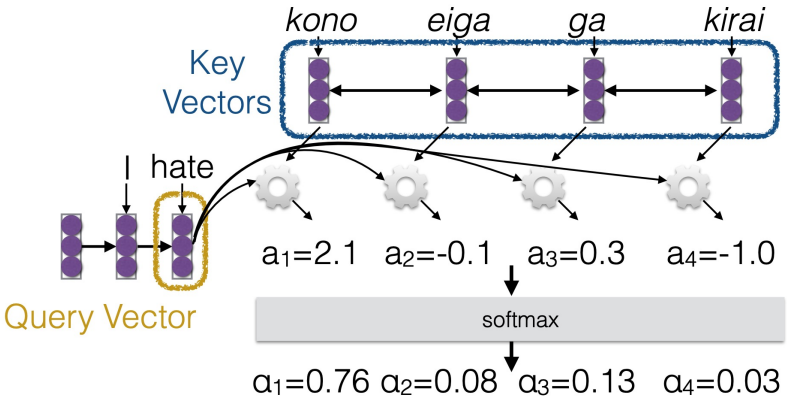
Calculating Attention

- Use “query” vector (decoder state) and “key” vectors (all encoder states)
- For each query-key pair, calculate weight
- Normalize to add to one using softmax



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Calculating Attention

- Combine together value vectors (usually encoder states, like key vectors) by taking the weighted sum

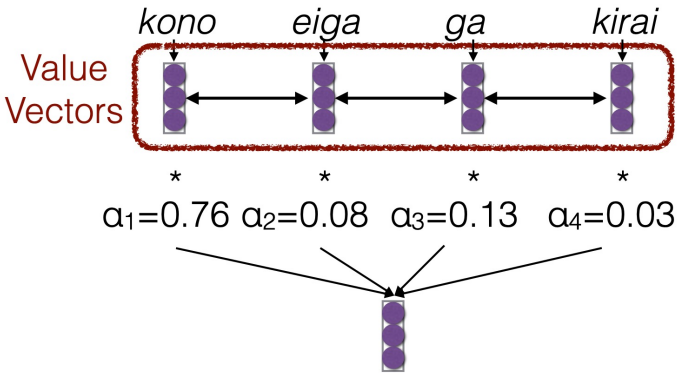

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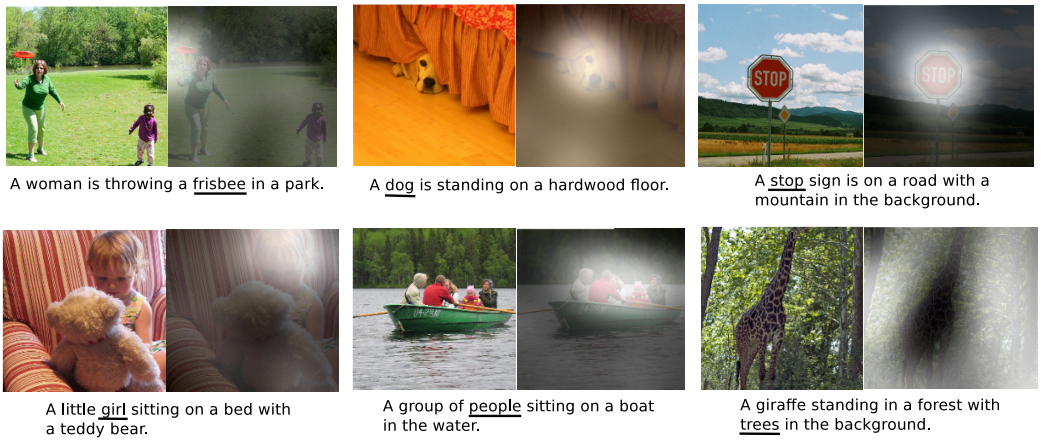
Image caption generation using attention



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

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Image caption generation using attention

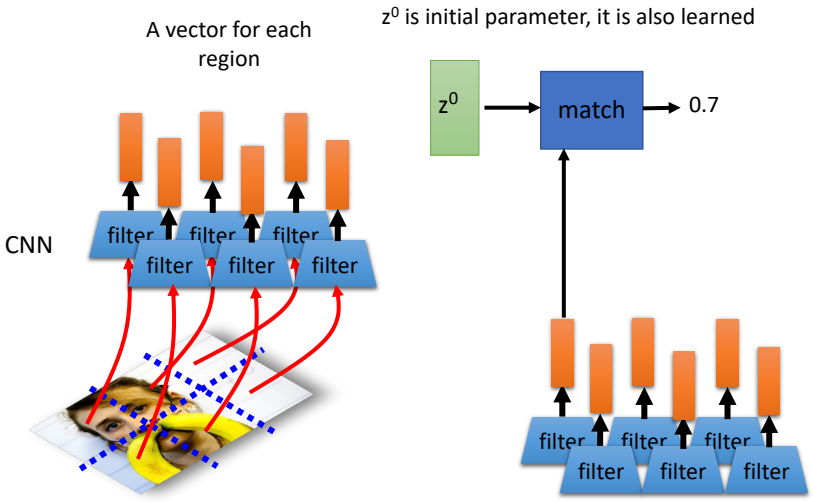

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Image caption generation using attention

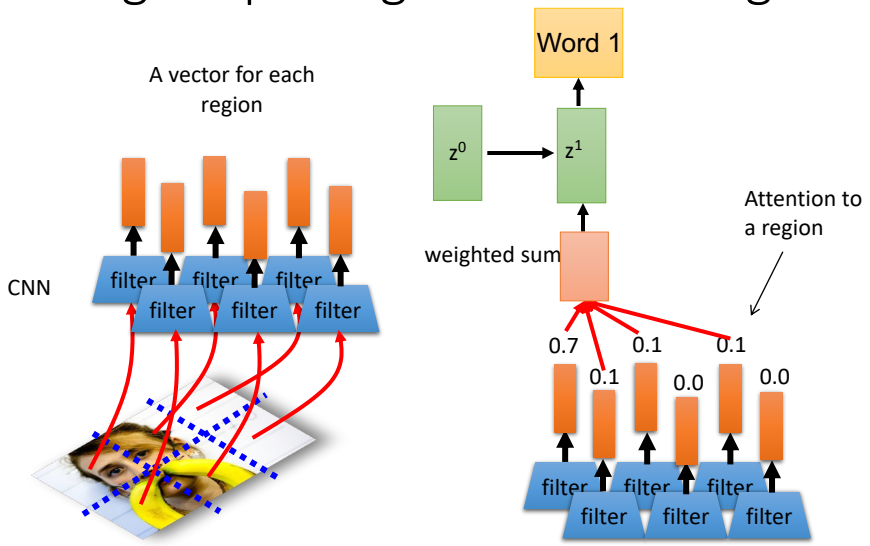

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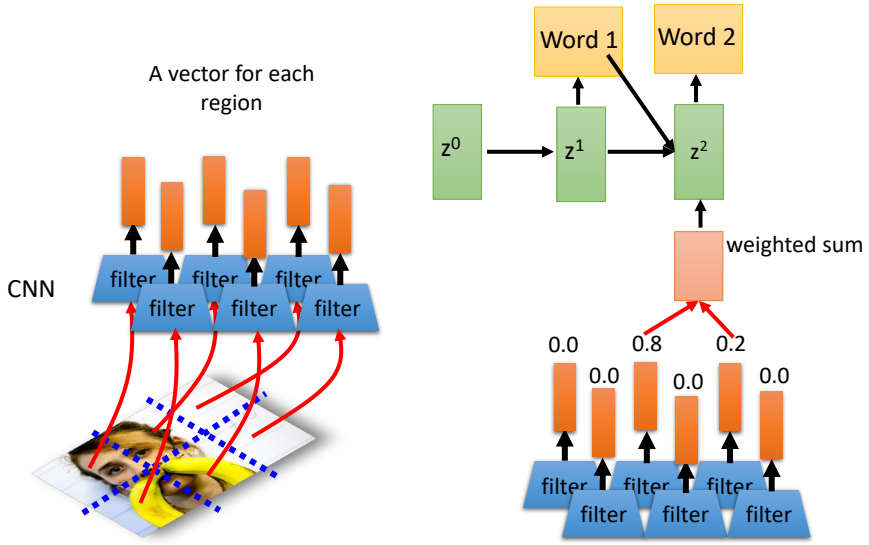
Image caption generation using attention



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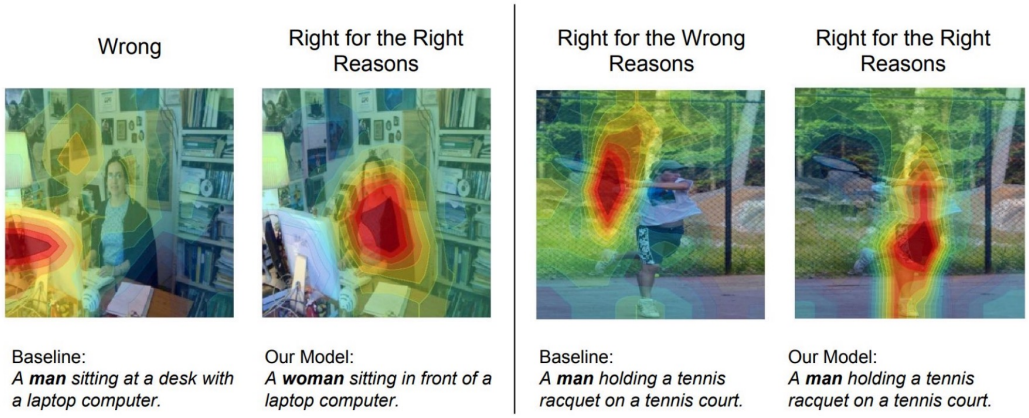
Attention can detect Gender Bias



Burns et al. "Women also Snowboard: Overcoming Bias in Captioning Models" ECCV 2018

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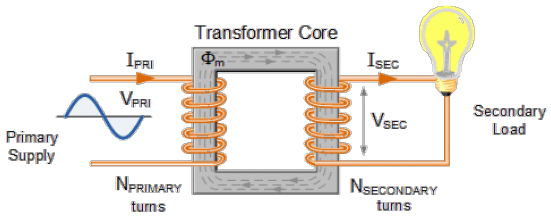
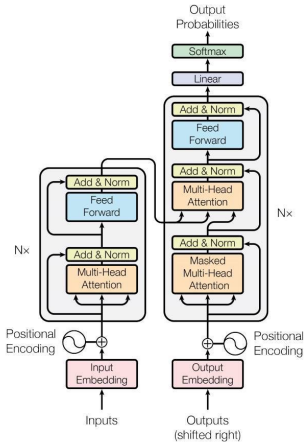
Transformers?





A neural network!!!

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Introduction

Attention Is All You Need

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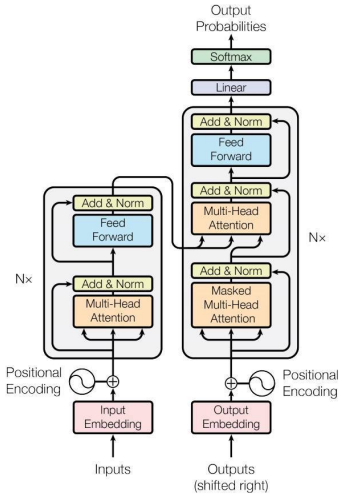

Vaswani, Ashish, et al. "Attention is All you Need." NeurIPS. 2017.

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Overview

- Input: A sentence in one language,
- Output: Translation in another.

https://jalammar.github.io/illustrated-transformer/ (slides come from this source)

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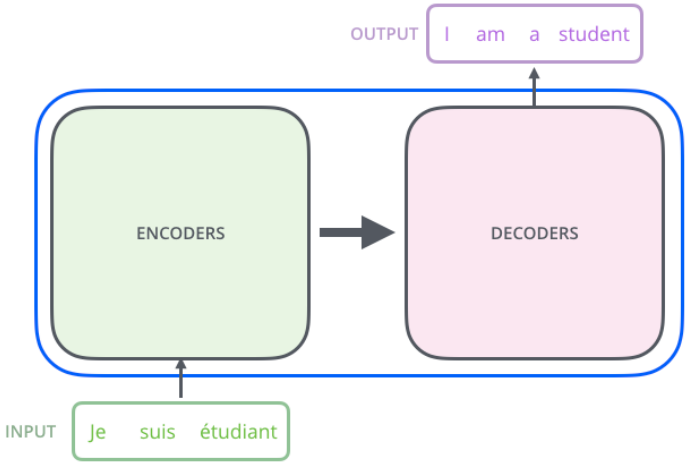
- A encoder-decoder model



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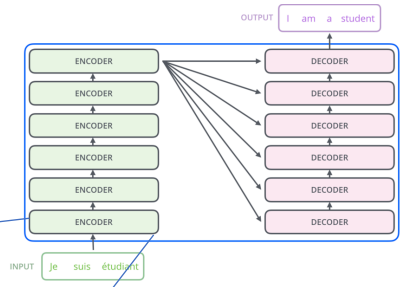
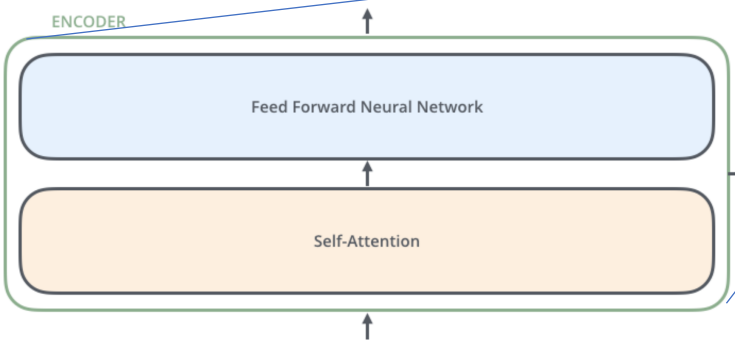
The **encoders** are **all identical in structure** (yet they do not share weights). Each one is broken down into two sub-layers





outputs of the self-attention are fed to a feed-forward neural network. The exact same one is independently applied to each position.

helps the encoder look at other words in the input sentence as it encodes a specific word.

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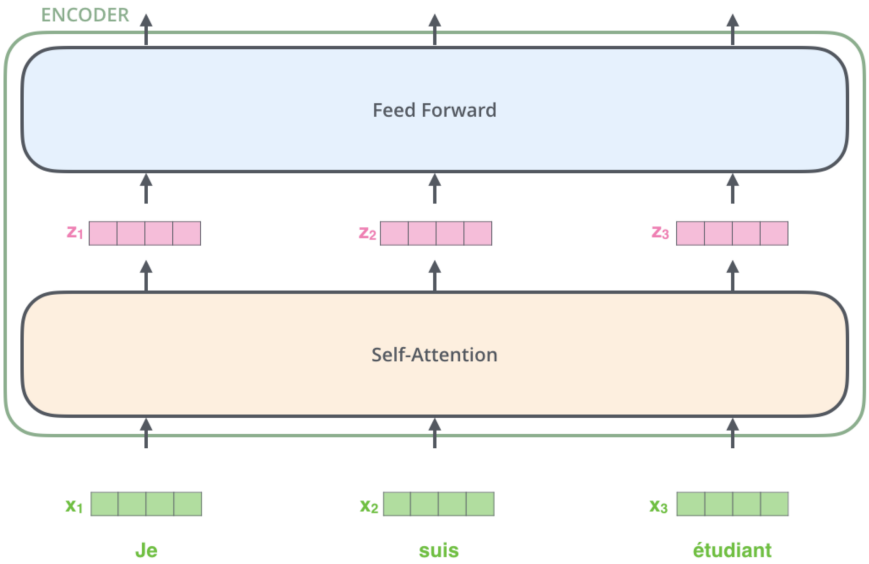
Key property of Transformer: word in each position flows through its own path in the encoder.

- There are dependencies between these paths in the self-attention layer.
- Feed-forward layer does not have those dependencies => various paths can be executed in parallel !



Word embeddings

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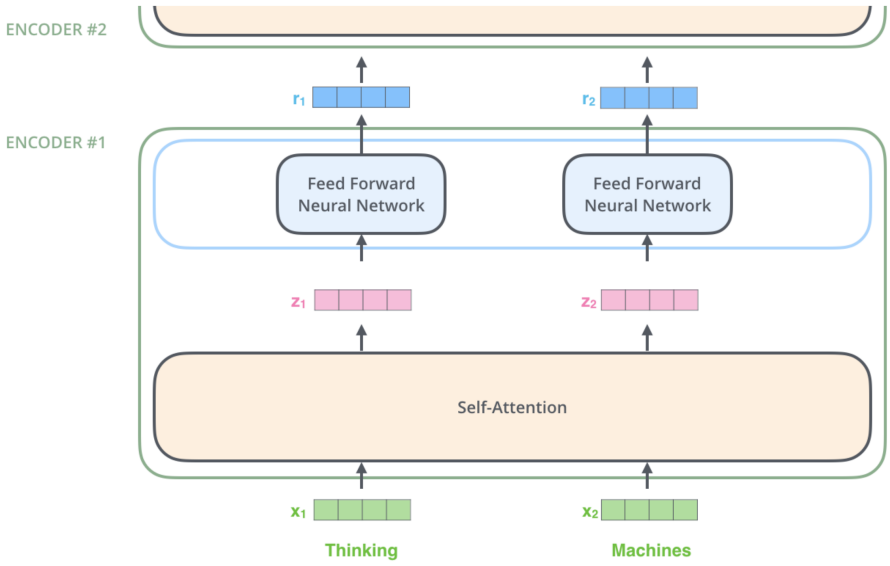
Visually clearer on two words

- dependencies in self-attention layer.
- No dependencies in Feed-forward layer



Word embeddings

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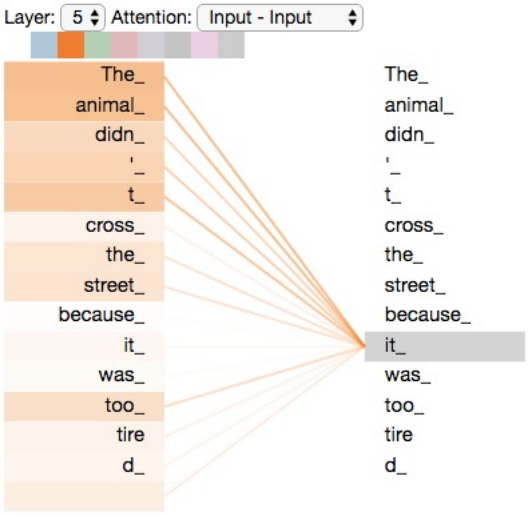
Self-attention

”The animal didn't cross the street because it was too tired”

What does “it” in this sentence refer to?



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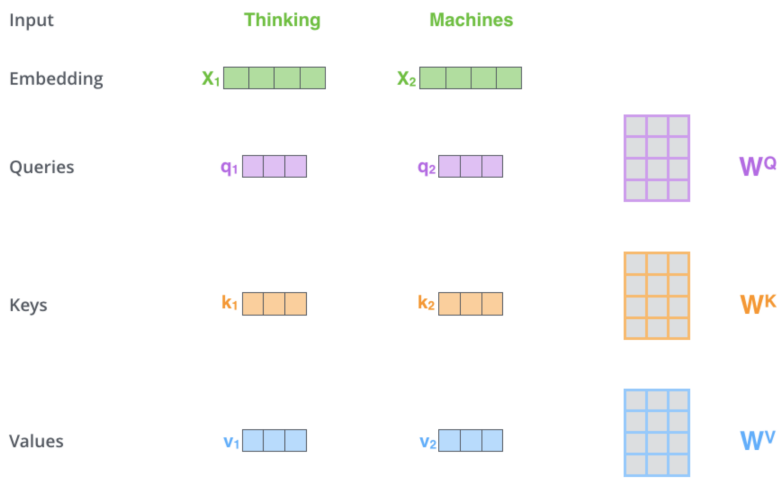
Self-Attention

While processing **each word** it allows to look at other positions in the input sequence for clues to build a better encoding for **this word**.

Step1: create three vectors from each of the encoder’s input vectors:

Query, Key, Value (typically smaller dimension).

by multiplying the embedding by three matrices that we **trained** during the training process.



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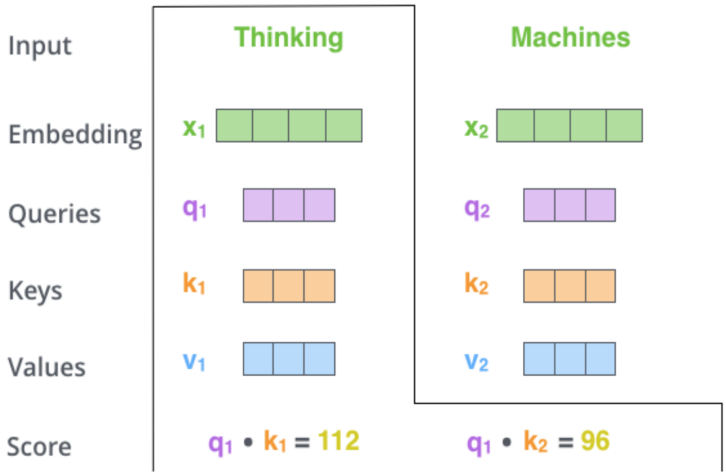
Self-Attention

Step 2: calculate a score (like we have seen for regular attention!) how much focus to place on other parts of the input sentence as we encode a word at a certain position.

Take dot product of the query vector with the key vector of the respective word we're scoring.



E.g., Processing the self-attention for word "Thinking" in position #1, the first score would be the dot product of q1 and k1. The second score would be the dot product of q1 and k2.

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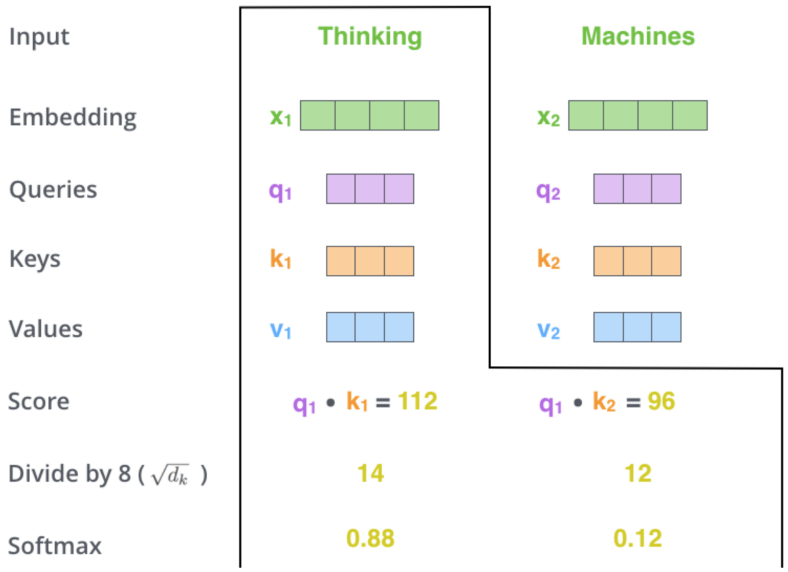
Self-Attention

- **Step 3** divide scores by the square root of the dimension of the key vectors (more stable gradients).
- **Step 4** pass result through a softmax operation. (all positive and add up to 1)



Intuition: softmax score determines how much each word will be expressed at this position.

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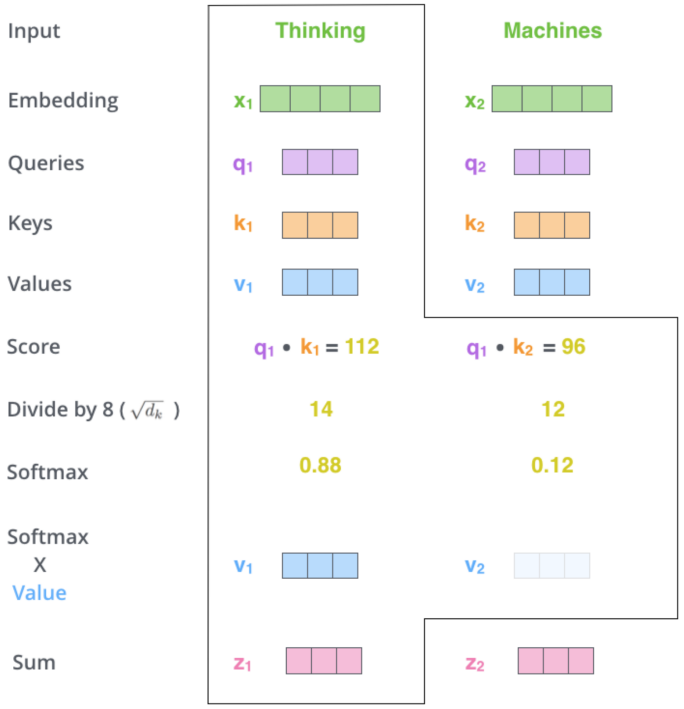
Self-Attention

- **Step5:** multiply each value vector by the softmax score (in preparation to sum them up).
- **Step6** : sum up the weighted value vectors. This produces the output of the self-attention layer at this position

More details:

- What we have seen for a word is done **for all words** (using matrices)
- Need to **encode position** of words
- And improved using a mechanism called "**multi-headed**" attention

(kind of like multiple filters for CNN)



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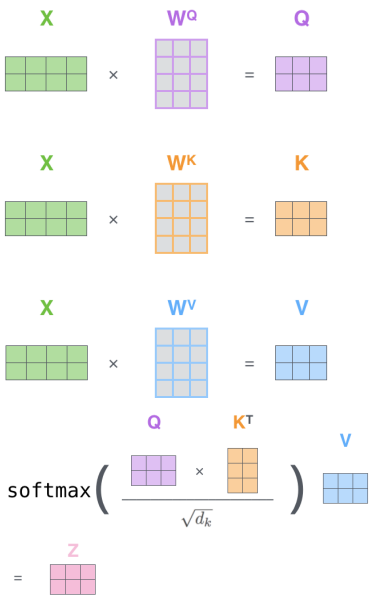
Matrix Calculation of Self-Attention

- **The first step** is to calculate the Query, Key, and Value matrices. We do that by packing our embeddings into a matrix X, and multiplying it by the weight matrices we've trained (WQ, WK, WV).

- **Then**, since we're dealing with matrices, we can condense steps two through six in one formula to calculate the outputs of the self-attention layer.



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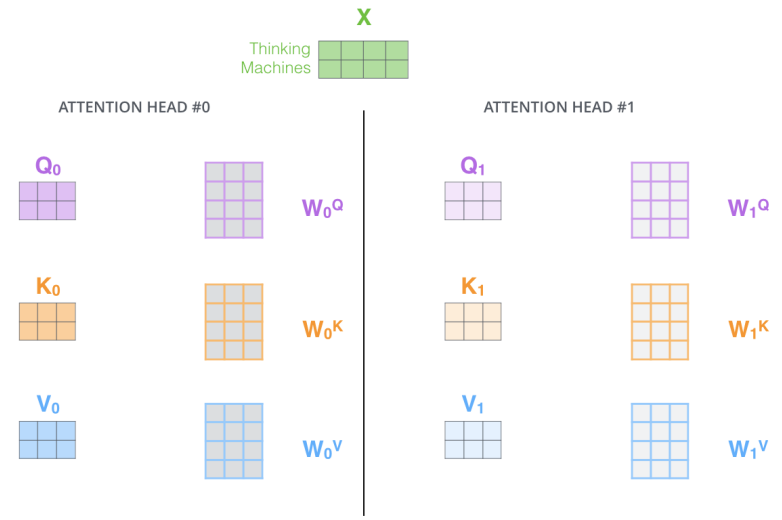
Multi-head self-attention

Why?

1. It expands the model's ability to focus on different positions.
2. It gives the attention layer multiple "representation subspaces".



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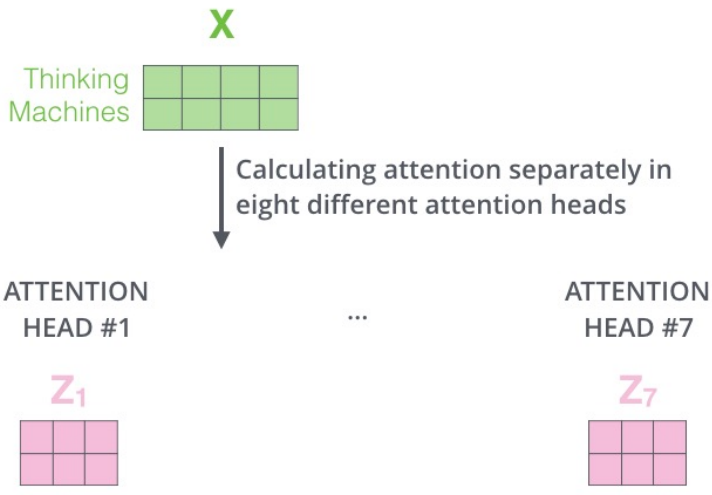

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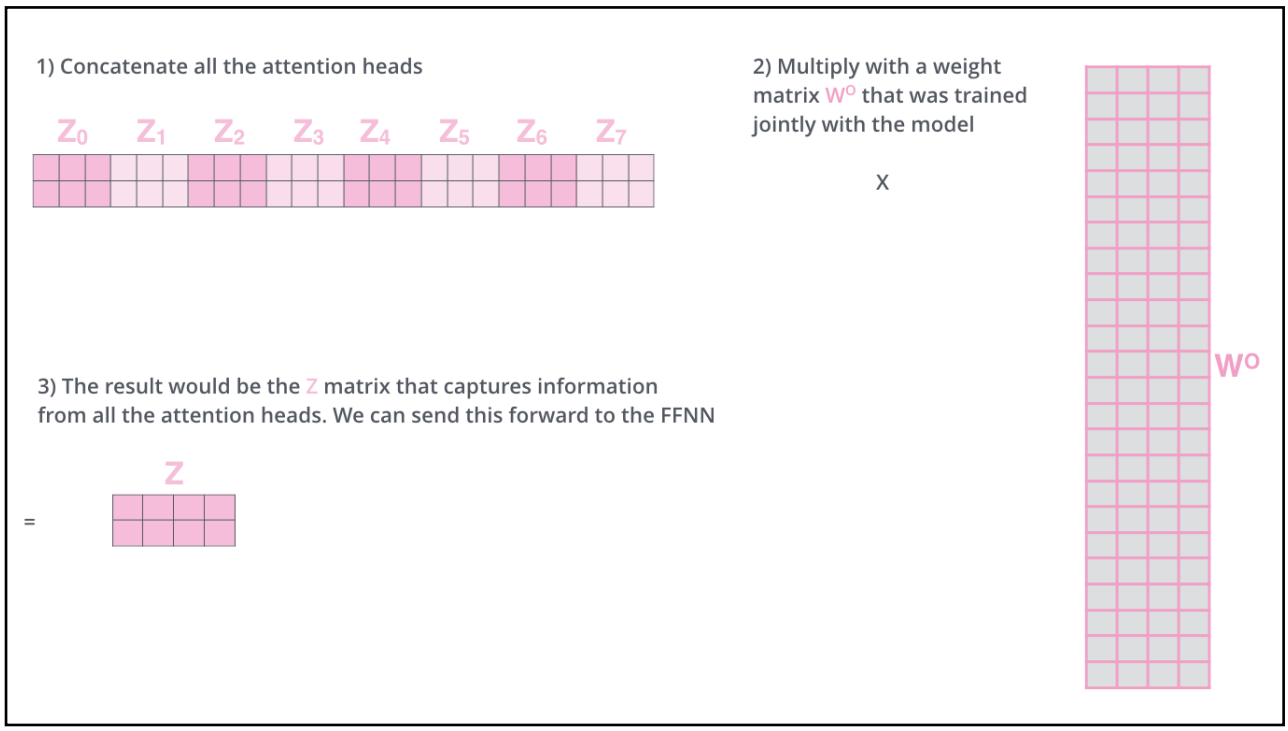
1) Concatenate all the attention heads
Z0 Z1 Z2 Z3 Z4 Z5 Z6 Z7
2) Multiply with a weight matrix WO that was trained jointly with the model
X
WO
3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN
=
Z

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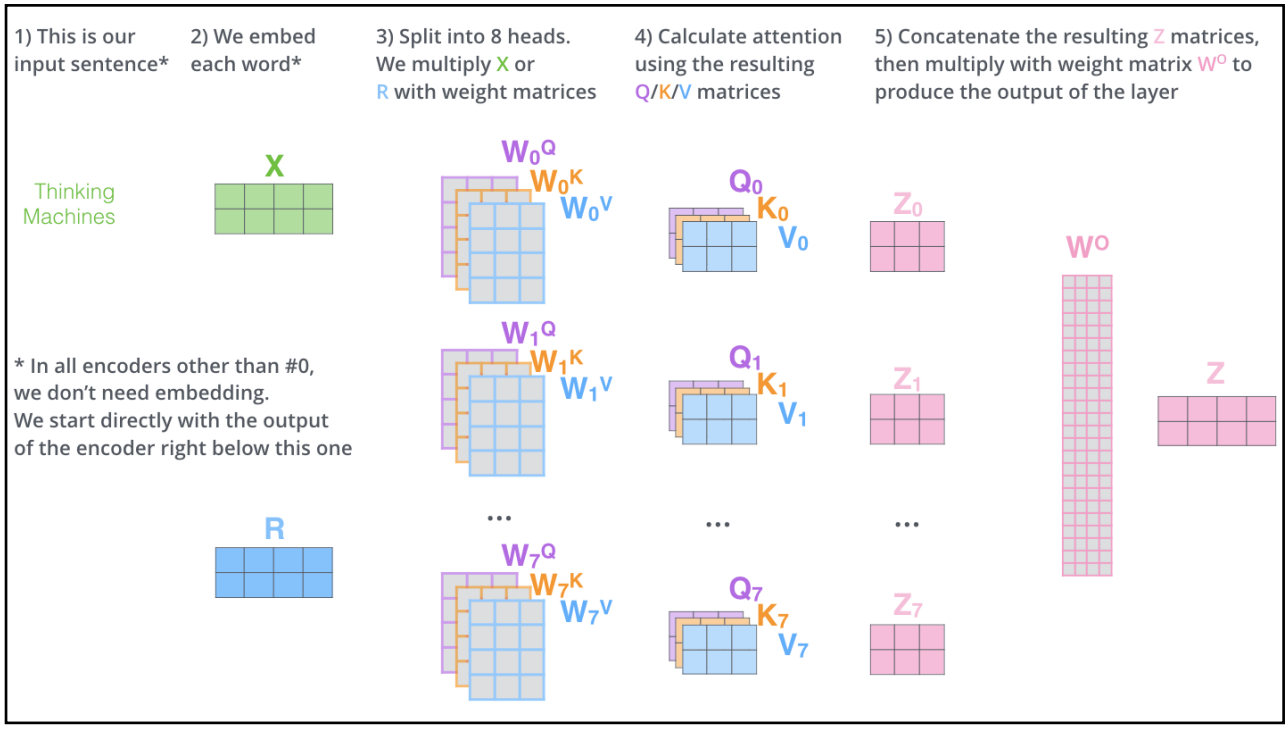
1) This is our input sentence*
2) We embed each word*
3) Split into 8 heads. We multiply X or R with weight matrices
4) Calculate attention using the resulting Q/K/V matrices
5) Concatenate the resulting Z matrices, then multiply with weight matrix WO to produce the output of the layer
Thinking Machines
X
W0Q W0K W0V
Q0 K0 V0
Z0
WO
Z
* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one
W1Q W1K W1V
Q1 K1 V1
Z1
R
...
W7Q W7K W7V
Q7 K7 V7
Z7

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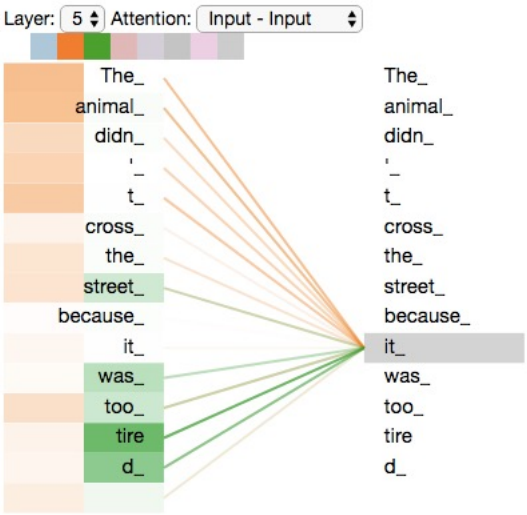

- As we encode the word "it" one attention head is focusing most on "the animal", while another is focusing on "tired" -- in a sense, the model's representation of the word "it" bakes in some of the representation of both "animal" and "tired".

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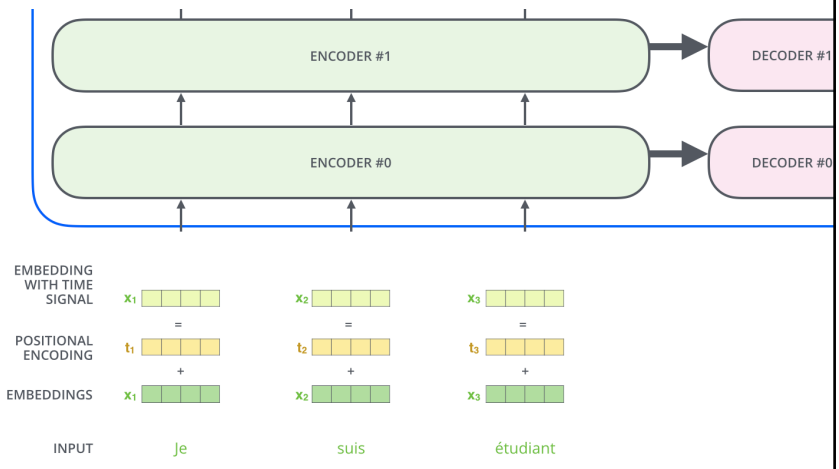
Position encoding

How to find a way to account for the order of the words in the input sequence?

Adds a vector to each input embedding.



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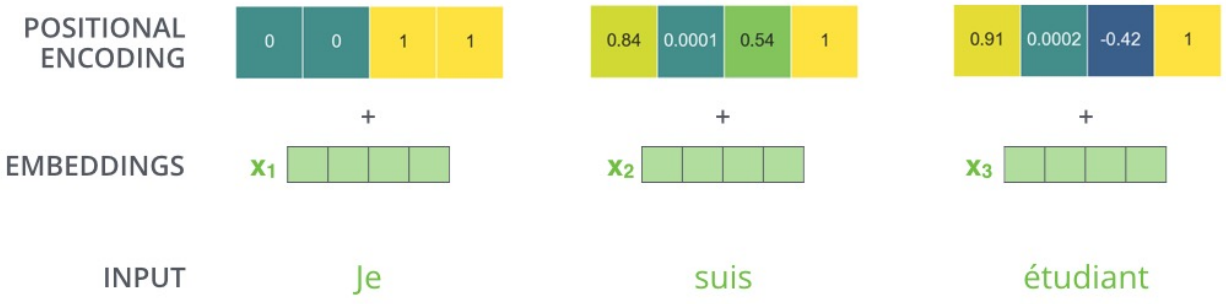
An example of position embedding

- Assume the embeddings has a dimensionality of 4:



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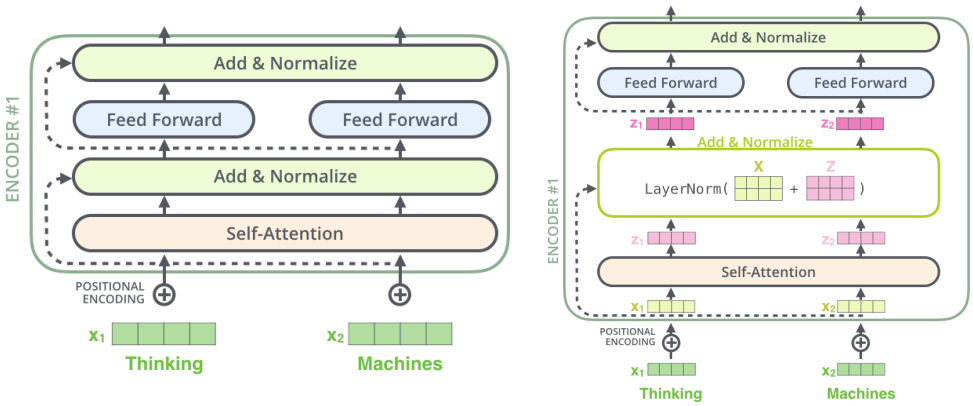
Residuals



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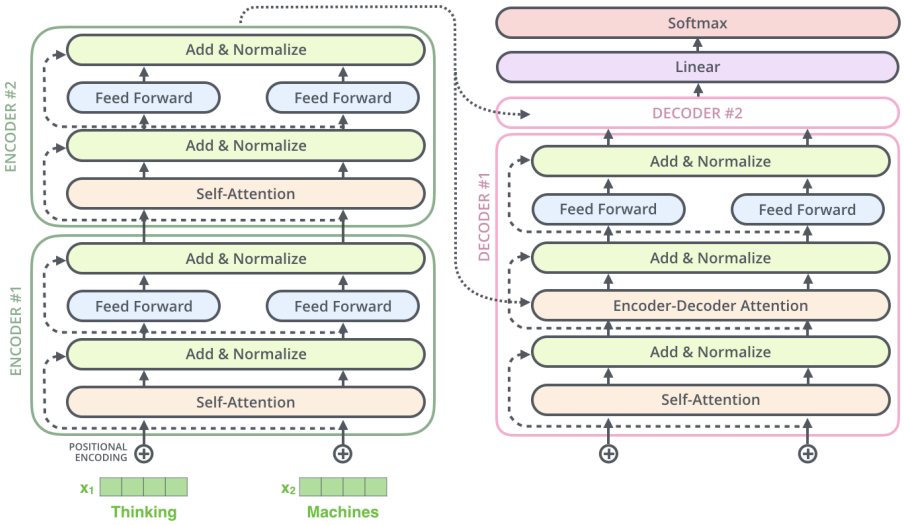
Residuals



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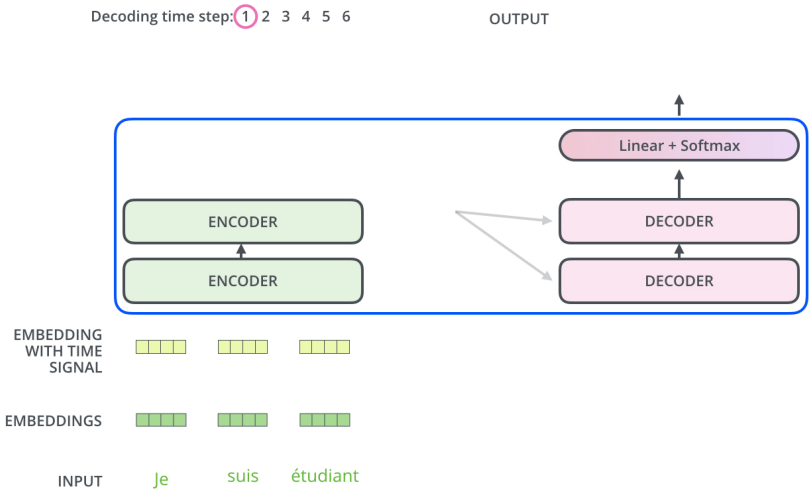
Decoder

In the decoder, the self-attention layer is only allowed to attend to earlier positions in the output sequence.



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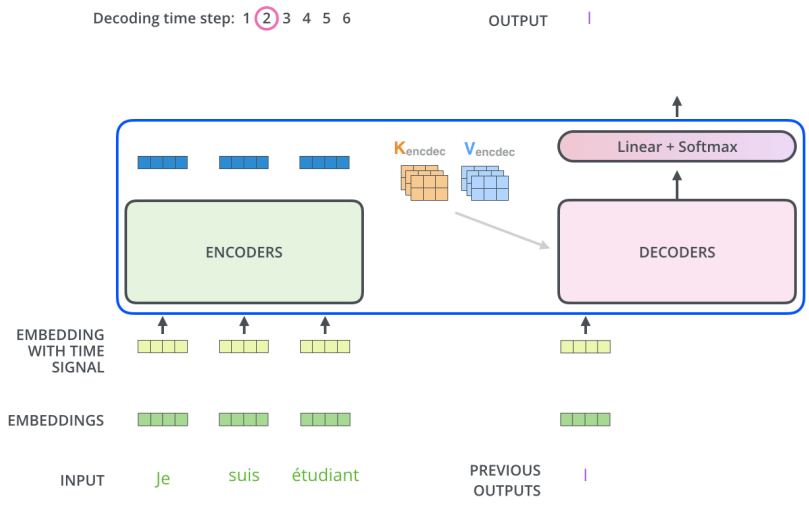
Decoder



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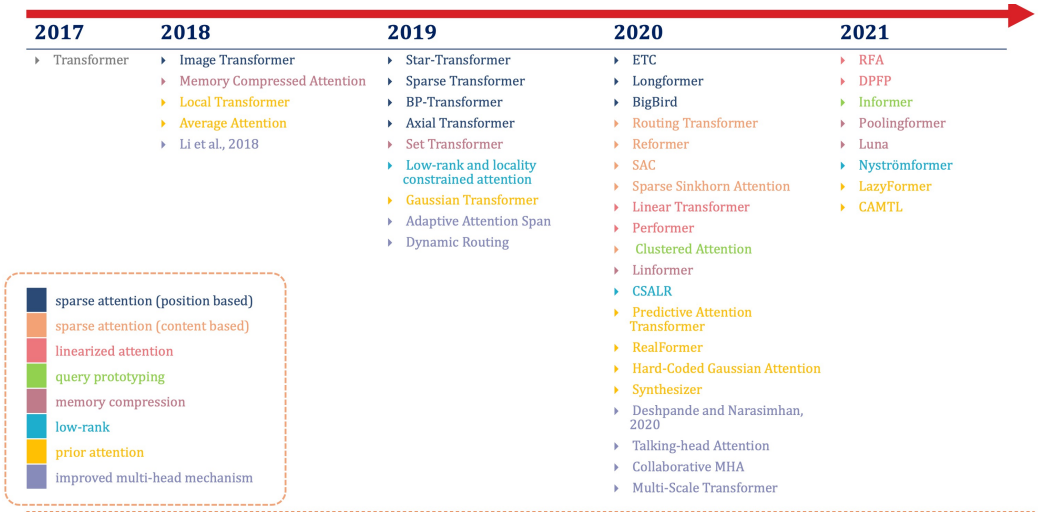
Transformer Variants



Picture from " A Tutorial of Transformers ", Xipeng Qiu

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Vision Transformer

From github.com/lucidrains/vit-pytorch

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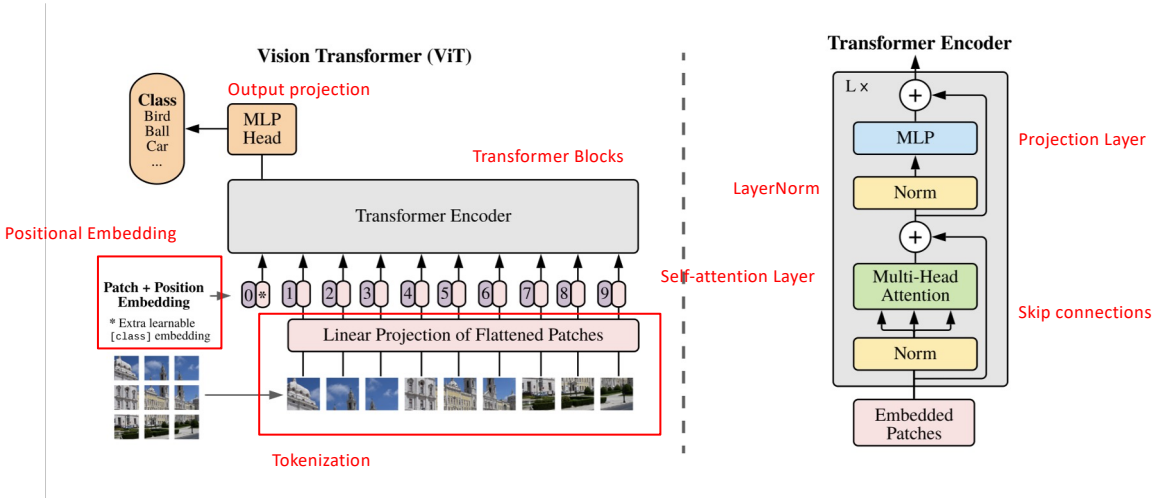
Vision Transformer



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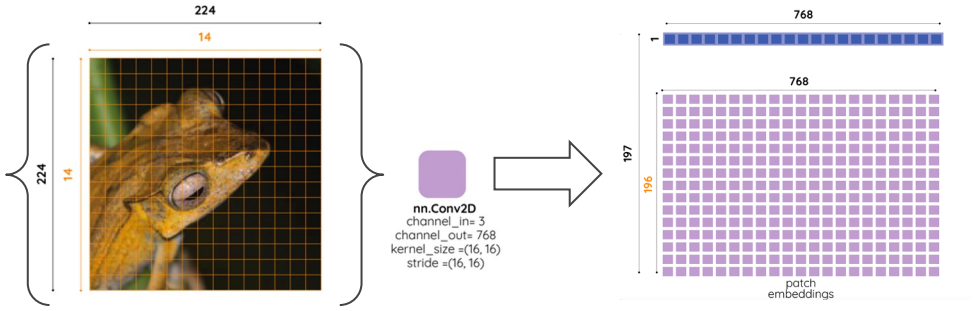
Tokenization

- Extracts non-overlapping image patches to create a **sequence** of tokens.
- Usually implemented as a Conv Layer (with stride equals kernel size), followed by Flattening
- [Optional] Class Token appended for classification tasks



From https://tugot17.github.io/Vision-Transformer-Presentation

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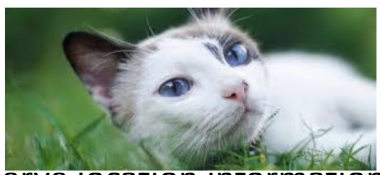
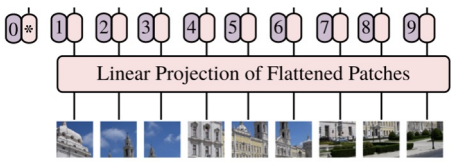
Positional Embedding

- The sequence of tokens are permutation invariant, a property which we do not want to have.



- To preserve location information of each token, we add positional embedding (Usually, a learnable tensor in vision)



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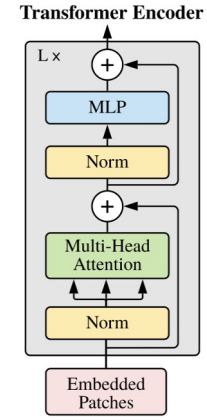
Transformer Block

- LayerNorm normalizes each token in channel dimension to give stability (Also, makes training stable even with small batch sizes).
- Multi-head Self-attention (MSA) computes pairwise attention using projected Key, Query and Value representations.
- Skip-connections help preserve/propagate structure among tokens.
- Projection Layers (MLPs) mix information within each token (among channels).



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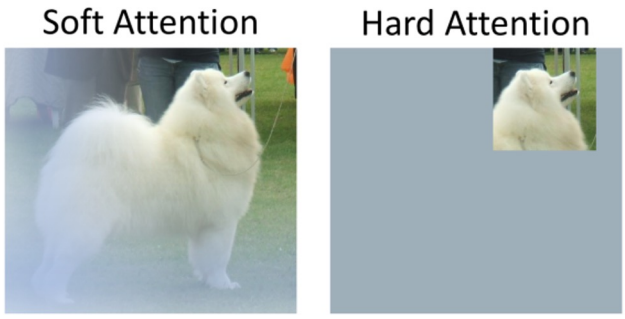
Spatial attention for images

Constraining(?) what goes into the CNN



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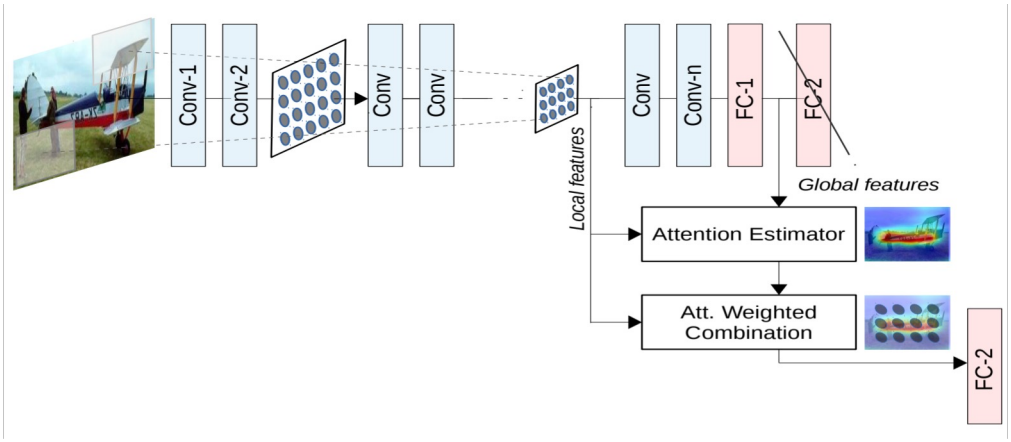
Spatial attention for images

Learn to generate a spatial weight matrix



1804.02391.pdf (arxiv.org)

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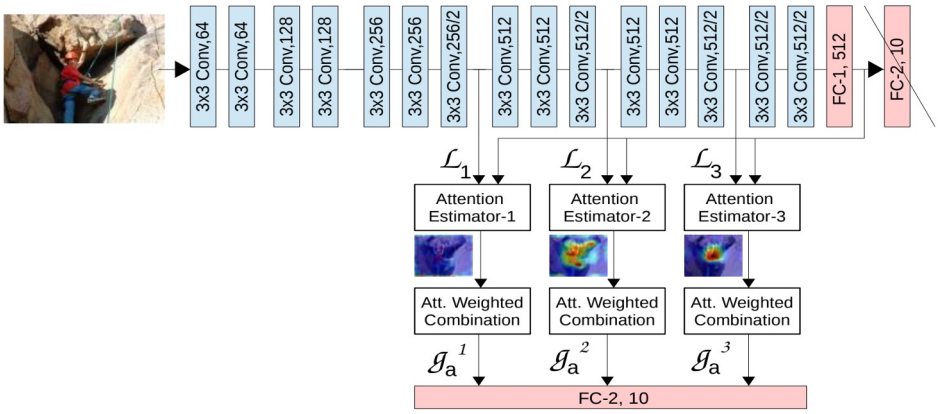
Spatial attention for images

Learn to generate a spatial weight matrix



1804.02391.pdf (arxiv.org)

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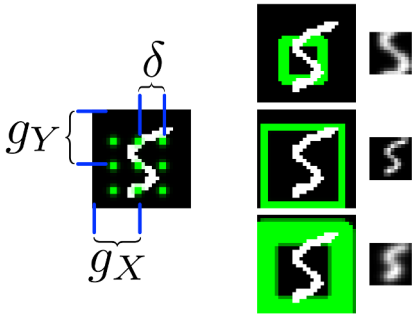
DRAW attention

Spatial attention for images

Representing attention in terms of few parameters



$$(\tilde{g}_X, \tilde{g}_Y, \log\sigma^2, \log\tilde{\delta}, \log\gamma) = W(h^{dec})$$

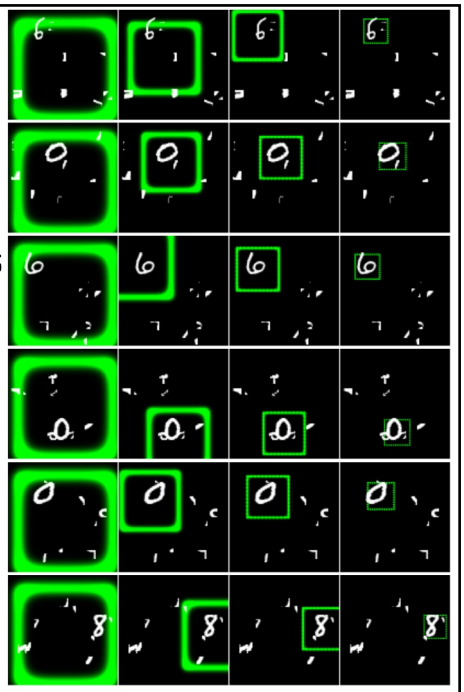
$$g_X = \frac{A+1}{2}(\tilde{g}_X + 1)$$

$$g_Y = \frac{B+1}{2}(\tilde{g}_Y + 1)$$

$$\delta = \frac{\max(A,B)-1}{N-1}\tilde{\delta}$$

$$F_X[i,a] = \frac{1}{Z_X}\exp\left(-\frac{(a-\mu_X^i)^2}{2\sigma^2}\right)$$

$$F_Y[j,b] = \frac{1}{Z_Y}\exp\left(-\frac{(b-\mu_Y^j)^2}{2\sigma^2}\right)$$



DRAW: A Recurrent Neural Network For Image Generation (arxiv.org)

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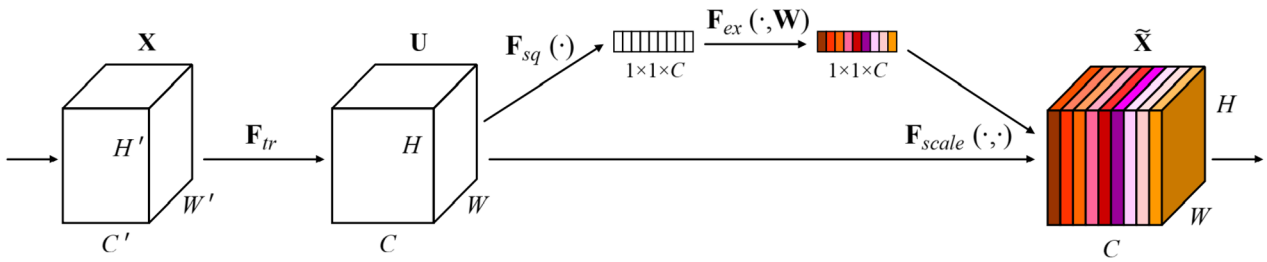
Other forms of attention

Channel-wise attention: Squeeze-and-Excitation network

- Learn to weigh/select channels



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Code for Vision Transformer

Pytorch Verision:

- https://github.com/rwightman/pytorch-image-models/blob/master/timm/models/vision_transformer.py
- https://github.com/lucidrains/vit-pytorch

TensorFlow Version:

- https://github.com/google-research/vision_transformer

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Recent Research on Vision Transformer

- Github Website: https://github.com/dk-liang/Awesome-Visual-Transformer
- Representative works: DeiT, Swin Transformer (ICCV 2021 Best Paper), BEIT, MAE, DiNO
- Different Task:

  Detection: DETR, CT3D

  Tracking: TransT, TrackFormer, STARK

  Segmentation: VisTR, Swin Transformer, Segmenter

  …

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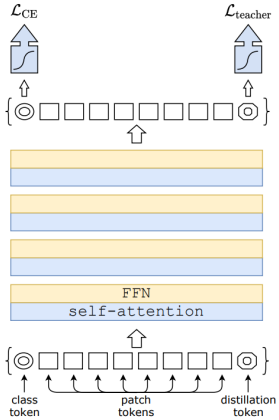
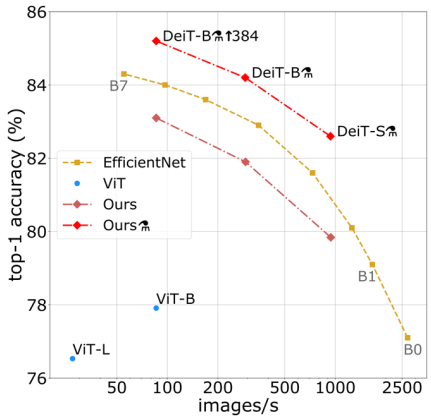
DeiT

Main idea:

Add a specific distillation token for Vision Transformer distillation Training





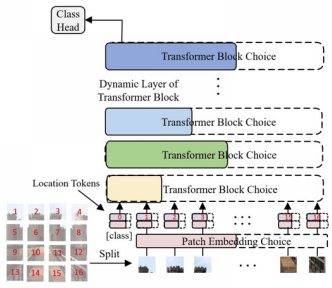
Touvron , Hugo, et al. "Training data-efficient image transformers & distillation through attention." ICML 2021.

61

AutoFormer

Main idea:

Search the optimal architecture of vision transformer with the proposed weight entanglement training strategy.



Chen , Minghao, et al. "AutoFormer: Searching Transformers for Visual Recognition." ICCV 2021.

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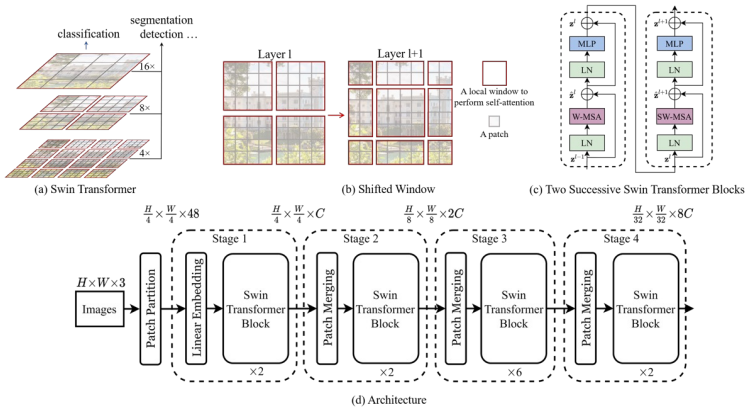
Swin Transformer

Main idea:

Design a hierarchical vision transformer macro architecture and compute the attention only on predefined windows. At last, use shifted window for information communication.



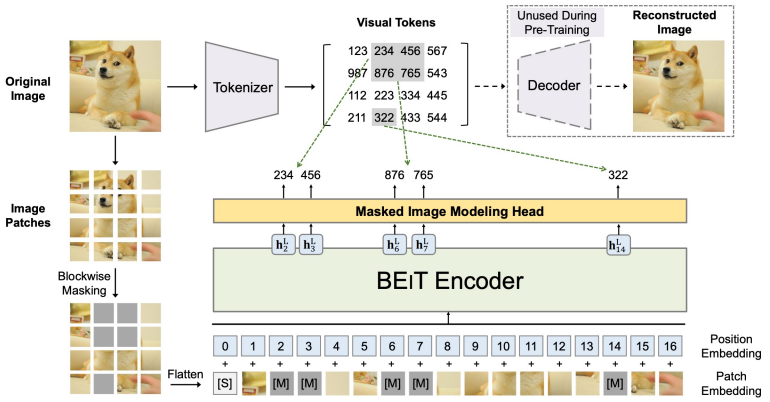
Liu, Zhe, et al. "Swin Transformer: Hierarchical Vision Transformer using Shifted Windows." ICCV 2021.

63

BEIT

Main idea:

"tokenize" the original image into visual tokens. Then, randomly mask some image patches and predict the labels.



Bao, hangbo et al. "BEiT: BERT Pre-Training of Image Transformers." ICLR 2022.

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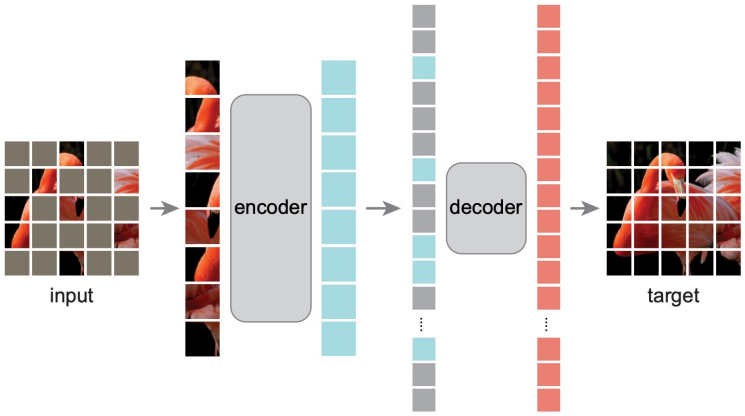
MAE

Main idea:

Mask random patches of the input image and reconstruct the missing pixels (pixel-level).

Encoder: Standard ViT

Decoder: Transformer Blocks



He, Kaiming et al. "Masked Autoencoders Are Scalable Vision Learners." CVPR 2022.

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