



Lecture 03: Transformer and its Application

Notes

- For the newly enrolled students, please select your top three favorite papers for in-class presentation:
(<https://docs.google.com/forms/d/e/1FAIpQLScxQ9Q3wCe7qEAW-qHO4cgC3L4-QKbSZn7VPVFZvOOwFhcOQQ/viewform>)
- We will try our best to fit.
- We use course website to post all the materials, brightspace is only used to post announcements and grades (<https://saiqianzhang.com/COURSE/>)
- You can find the in-class presentation formats, reading list assignments via the course website.

Recap

- Convolutional Neural Network
 - Basic building blocks
 - Popular CNN architectures
 - ResNet, MobileNet, ShuffleNet, SqueezeNet, DenseNet, EfficientNet, ConvNext, ShiftNet
 - CNN architectures for other Vision Tasks
 - Image Segmentation, Object Detection
- Recurrent Neural Network
 - Basic building blocks

Topics

- Transformer basics
- Vision transformer
- AIGC
 - LLM
- Self-supervised learning

Transformers

- Proposed in "Attention Is All You Need" in 2017
- The vanilla Transformer is a sequence-to-sequence model and consists of transformer blocks.

Attention Is All You Need

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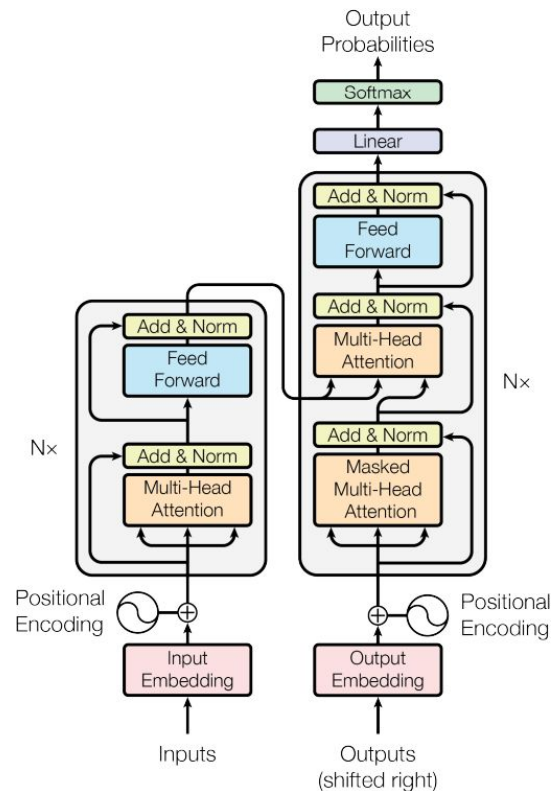
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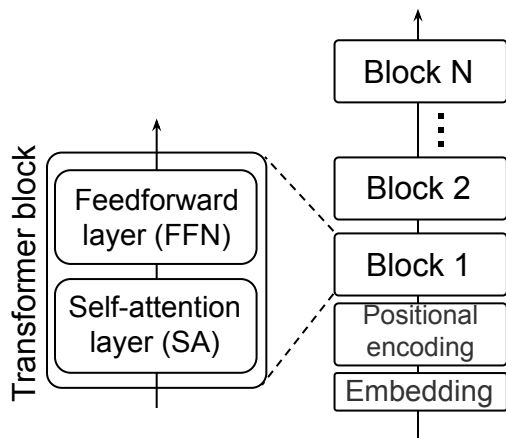
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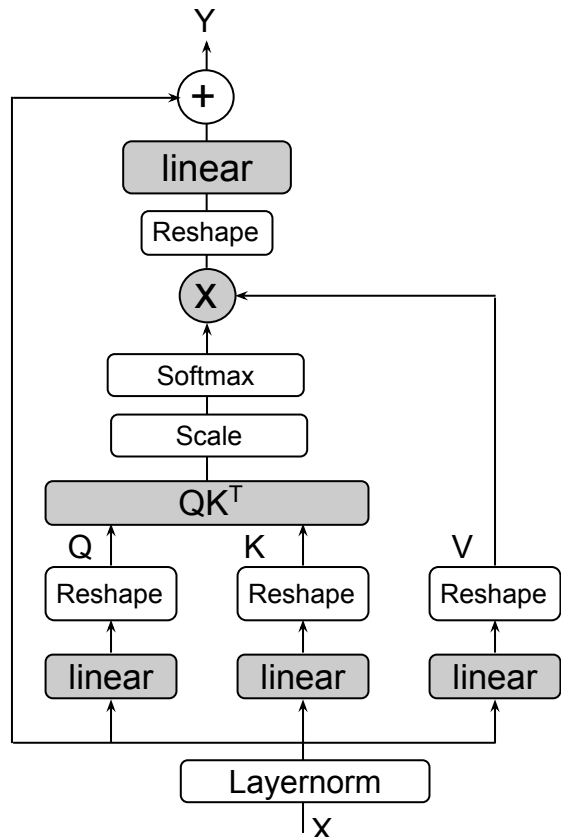
Illia Polosukhin* †
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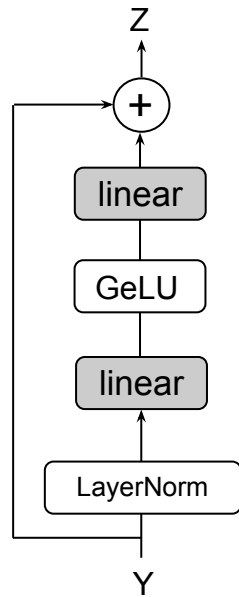
Transformers



- Each transformer block includes a self-attention layer and a feedforward layer.

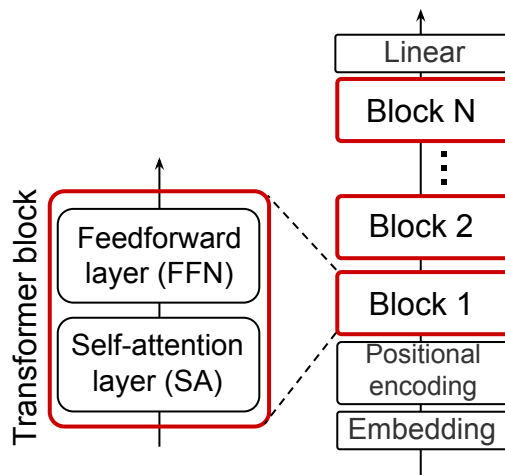


Self attention block (SA)

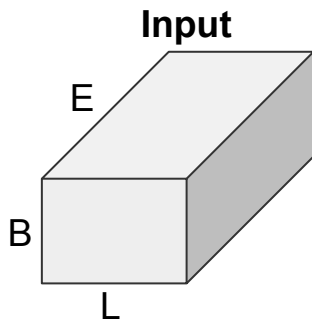


Feed forward block (FFN)

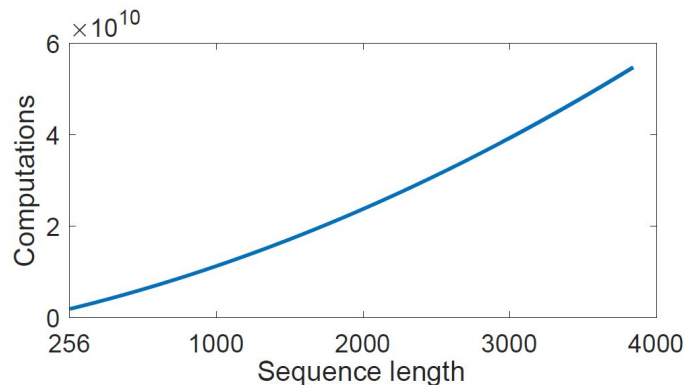
Transformers: Transformer Block



Transformers

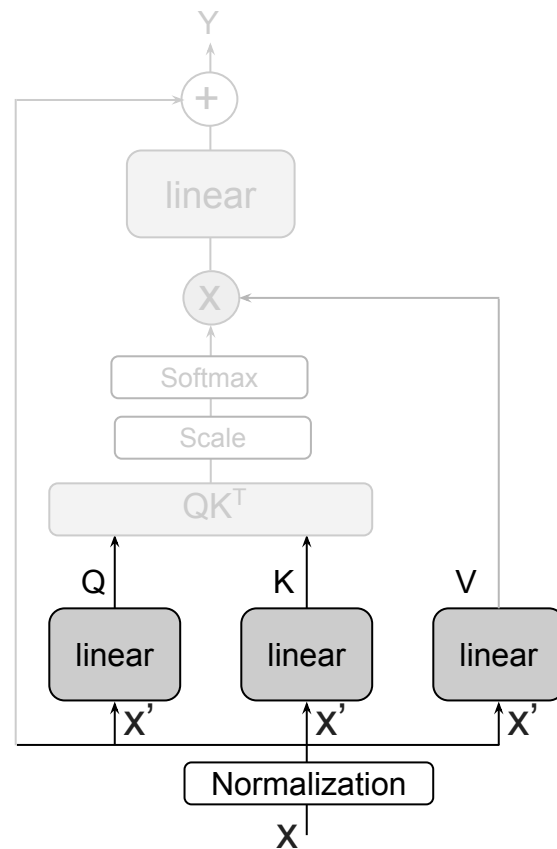


- The input contains three dimensions:
 - B: batch
 - L: token length
 - E: embeddings
- The amount of computation is closely related to the token length L.
- Longer sequences are disproportionately expensive because attention is quadratic to the sequence length.



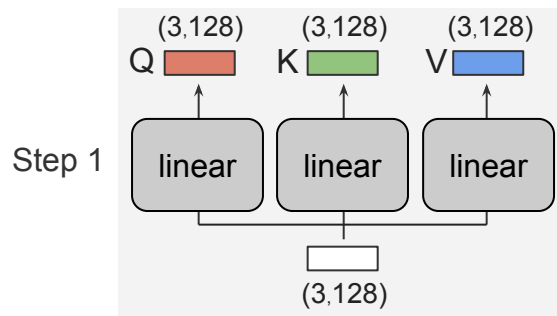
Self-Attention Block

- The input x is first normalized, then the first step in calculating self-attention is to create three vectors from the input x' , denoted as: Query (Q), Key (K), Value (V).
 - $(B, L, E) * (E * E) \rightarrow (B * L * E)$ (BLE^2)
- The second step in calculating self-attention. This will compute the attention score between each pair of input tokens.
 - $QK^T \rightarrow (B, L * E) * (B, E * L) \rightarrow (B, L * L)$
- Scale and normalize the score using softmax.
 - $\text{Softmax}(QK^T) \rightarrow (B, L * L)$
- Multiply each value vector by the softmax score.
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 - $(B, L * L) * (B, L * E) \rightarrow (B, L * E)$
- Pass the result to the linear layer, sum with the input.



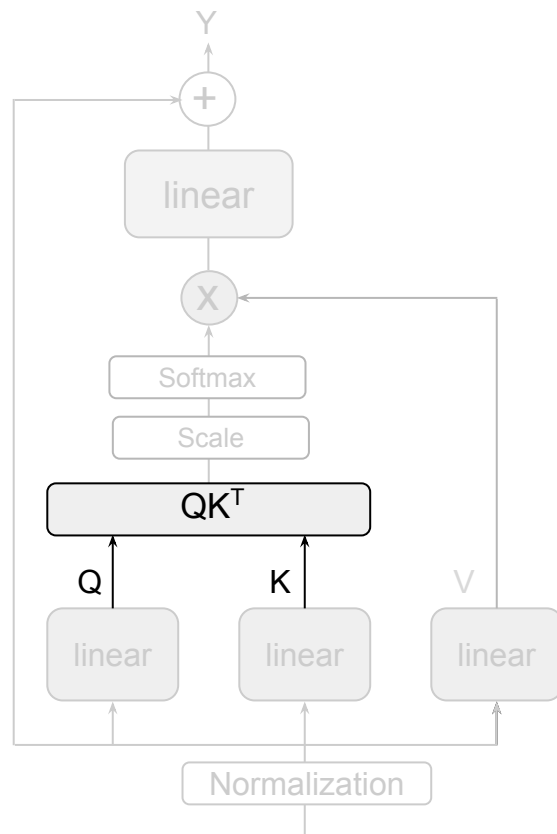
Example

“I love AI” \longrightarrow 3 $\begin{matrix} 128 \\ \square \end{matrix}$



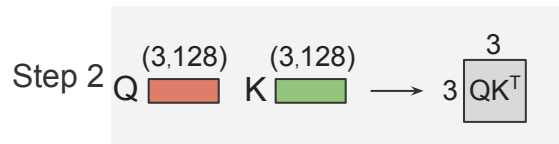
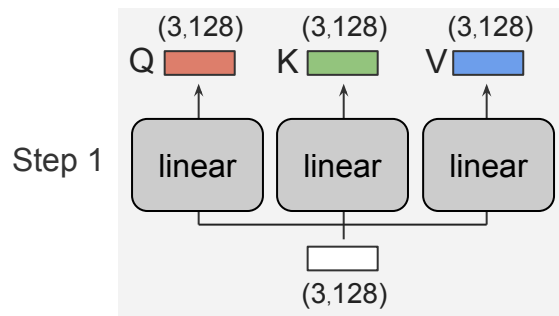
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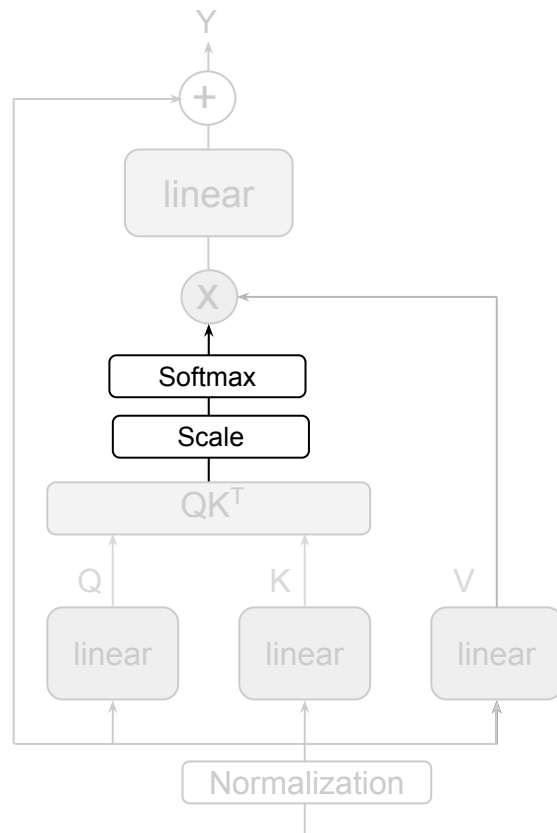
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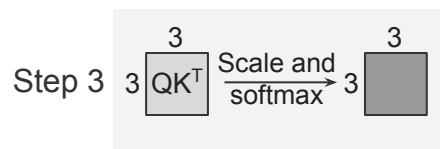
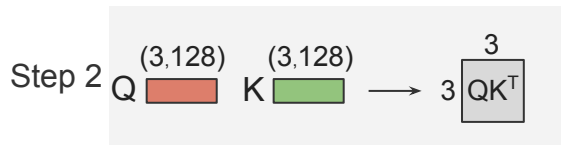
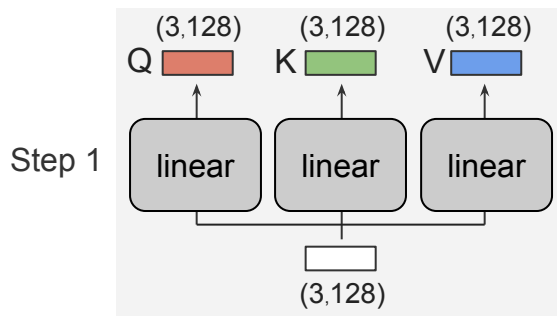
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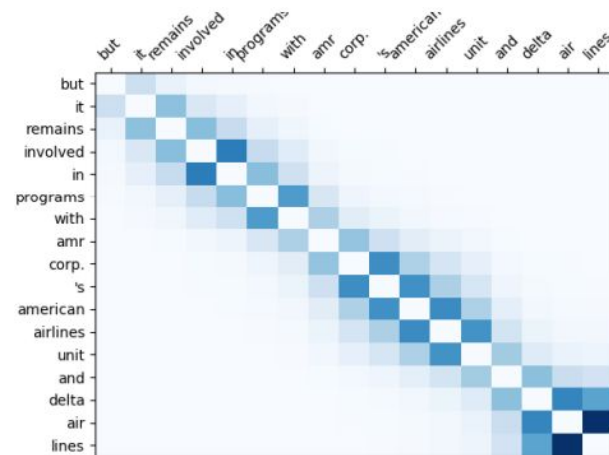
Example

“I love AI” \longrightarrow 3×128



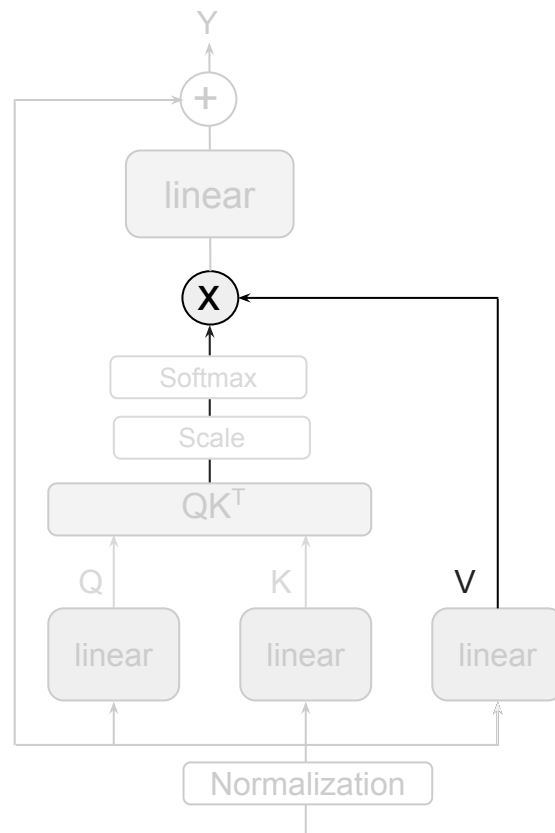
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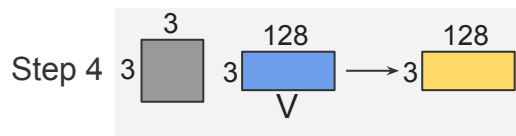
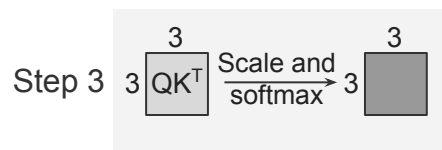
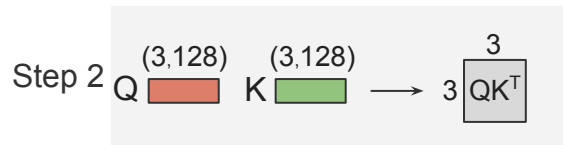
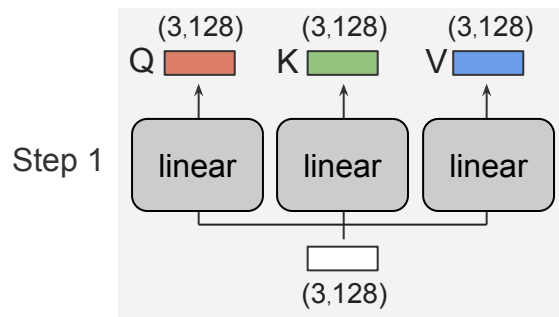
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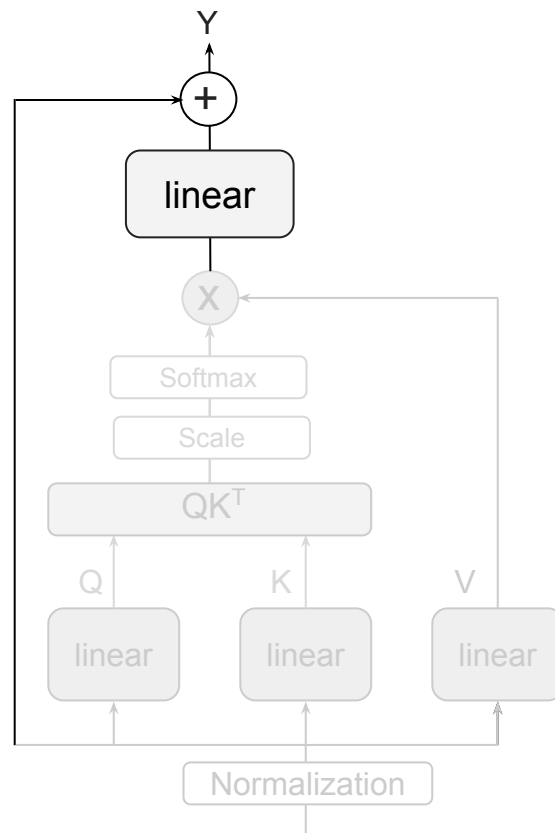
Example

“I love AI” \longrightarrow 3×128



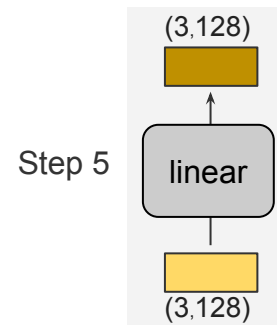
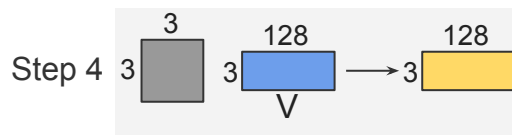
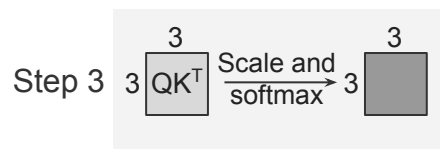
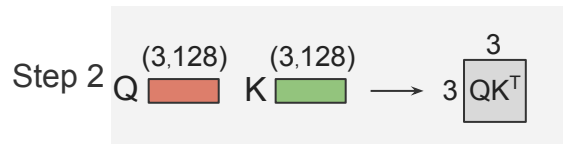
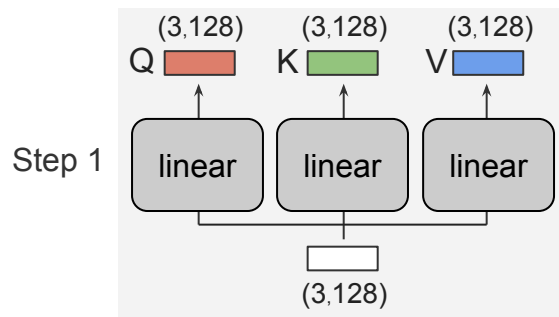
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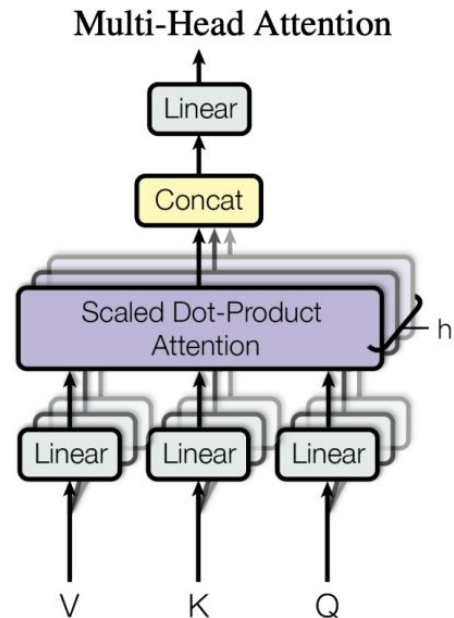
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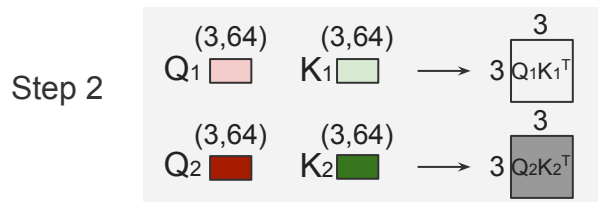
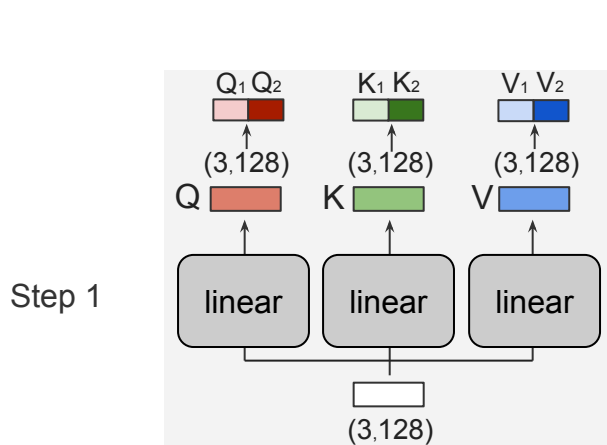


Multi-headed Attention

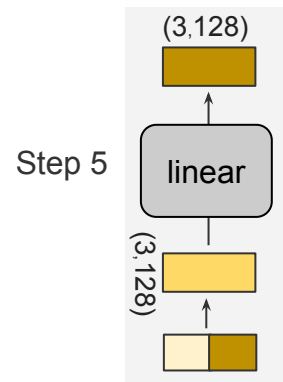
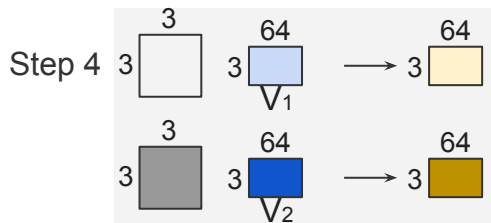
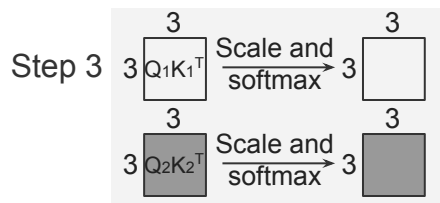
- Q, K, V tensors are broken into multiple components along the embedding dimension.
 - $(B, L, E) \times (E \times E) \rightarrow (B \times L \times E)$
 - $(B, L, E) \rightarrow (B, M, L, E/M) \rightarrow (B, M, L, D)$, where $D=E/M$
- All the following operations can be performed independently over each head M .
 - $QK^T \rightarrow (B, M, L \times D) \times (B, M, D \times L) \rightarrow (B, M, L \times L)$
 - $\text{Softmax}(QK^T) \rightarrow (B, M, L \times L)$
 - $\text{Softmax}(QK^T) \times V \rightarrow (B, M, L \times L) \times (B, M, L \times D) \rightarrow (B, M, L \times D) \rightarrow (B \times L \times E)$



Example

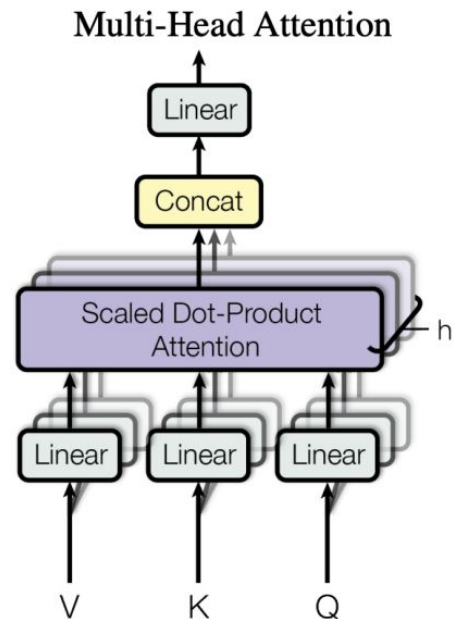


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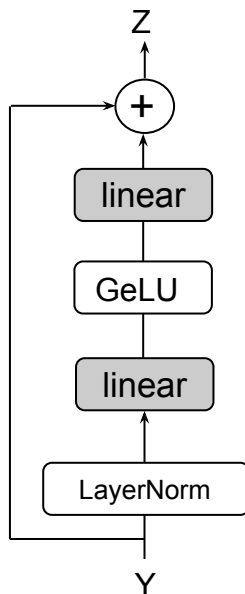


Multi-headed Attention

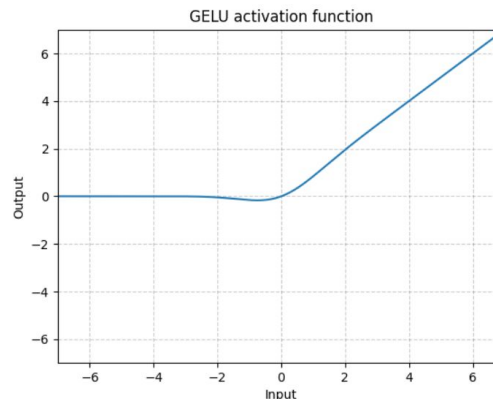
- Why we need multiple heads?
 - Multiple attention heads in transformers are used to enhance the expressive power and modeling capabilities of the network.
 - By using multiple attention heads, transformers can capture different types of dependencies and relationships between words or elements in a sequence.
 - Having multiple heads allows the model to perform attention calculations in parallel, which can improve computational efficiency.



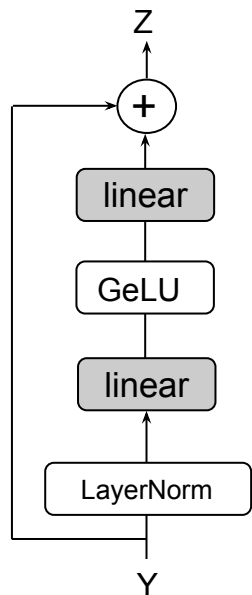
Feed Forward Layer



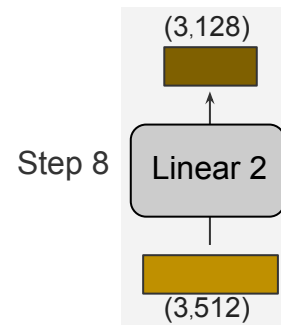
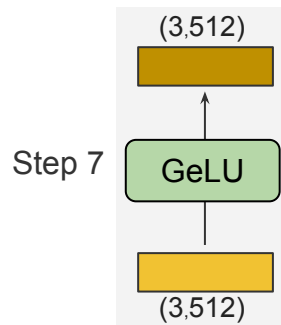
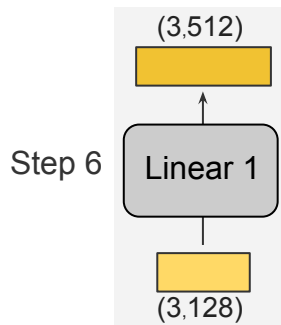
- The two linear layers are big:
 - $(Ex4E)$ and $(4ExE)$, E can be large (e.g., 4096)
 - This is expensive to implement.
- GeLU:
 - $GeLU(x) = x\Phi(x)$
 $\Phi(x) = P(y \leq x)$, where $Y \sim N(0, 1)$



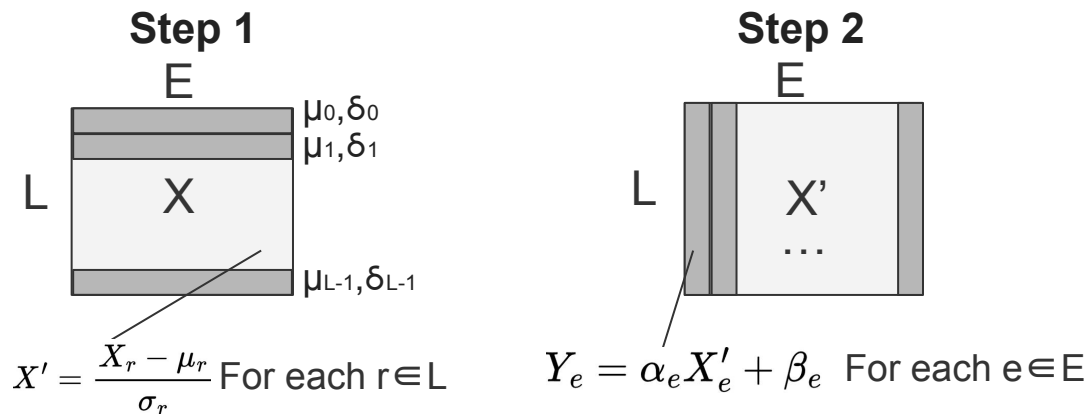
Example



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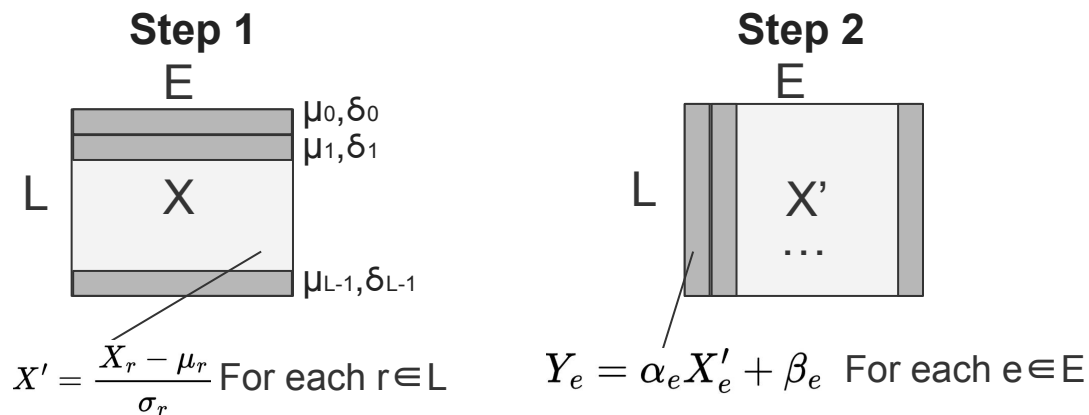


Layer Normalization



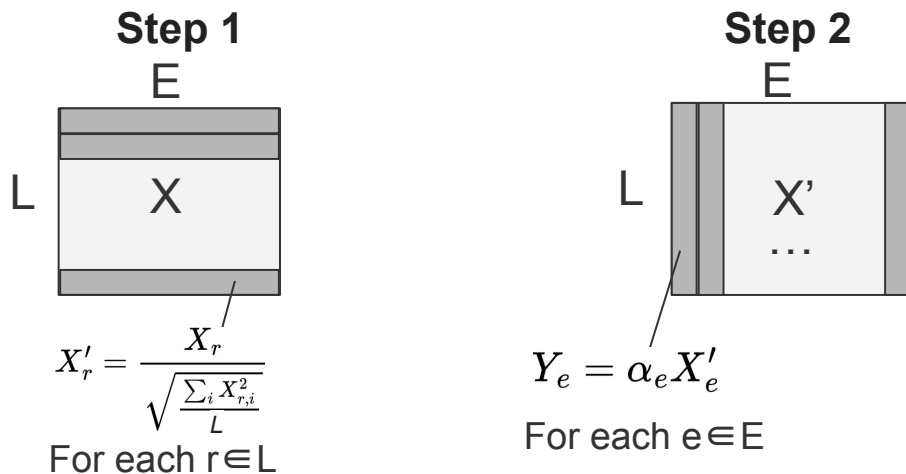
- LayerNorm is applied on each input sample.
- Both α and β have a length of E .

Layer Normalization



- Layer Norm does not store the running mean and running variance, so during the inference time, the mean and variance need to be computed.

RMS Normalization



- The experiments demonstrate RMSNorm achieves similar and even better results than LayerNorm.

Transpose & Reshape

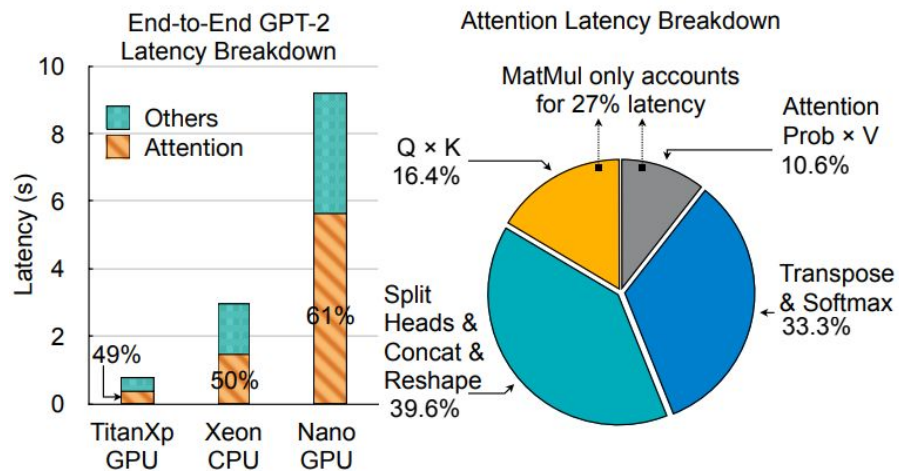


Fig. 2. End-to-End GPT-2 latency breakdown on various platforms, and attention latency breakdown on TITAN Xp GPU. Attention accounts for over 50% of total latency. Data movements account for 73% of attention latency.

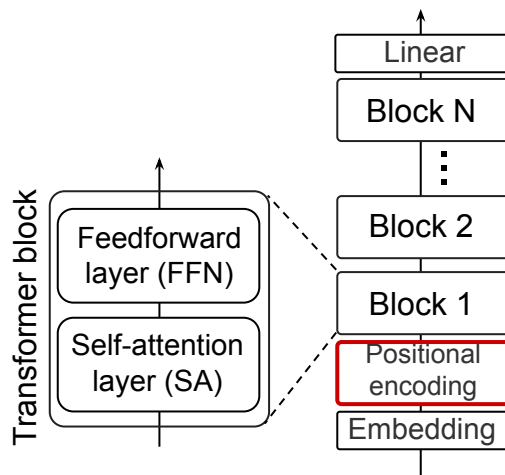
Reshaping operation

$$(B, L, E) \longrightarrow (B, M, L, E/M)$$

Transpose operation

$$(B, L, E) \longrightarrow (B, E, L)$$

Transformers: Positional Encoding



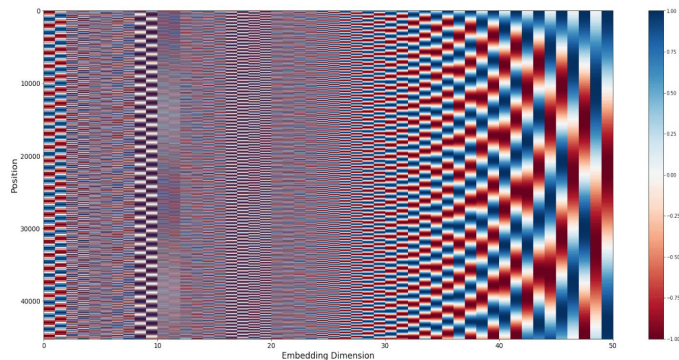
Transformers: Positional Encoding

- One thing that's missing from the model as we have described it so far is a way to account for the order of the words in the input sequence.
- Transformer adds a vector to each input embedding. These vectors follow a specific pattern that the model learns, which helps it determine the position of each word.

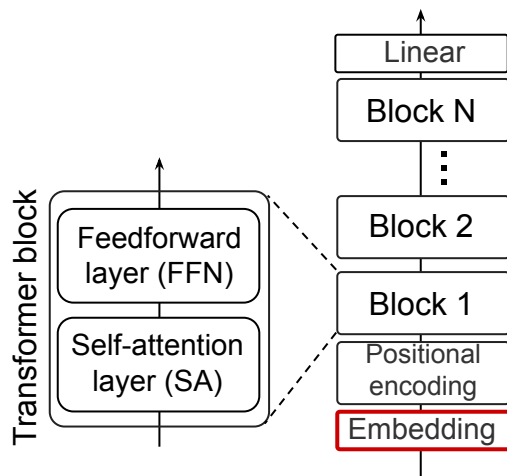
$$PE_{(pos,2i)} = \sin(pos/10000^{2i/d_{\text{model}}})$$

$$PE_{(pos,2i+1)} = \cos(pos/10000^{2i/d_{\text{model}}})$$

- For long sequences, the indices can become quite large. Normalizing these index values to a range between 0 and 1 can cause issues with variable-length sequences, as each sequence would be normalized differently.
- pos is the positional of the token, i is the index of the embedding.

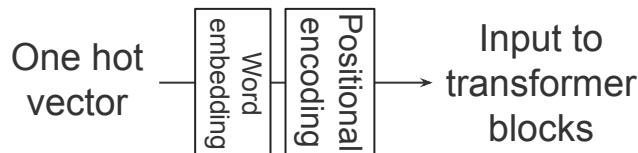
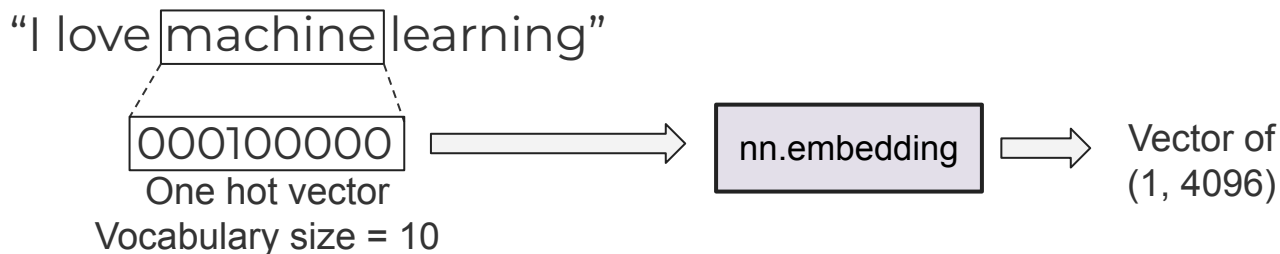


Transformers: Word Embedding



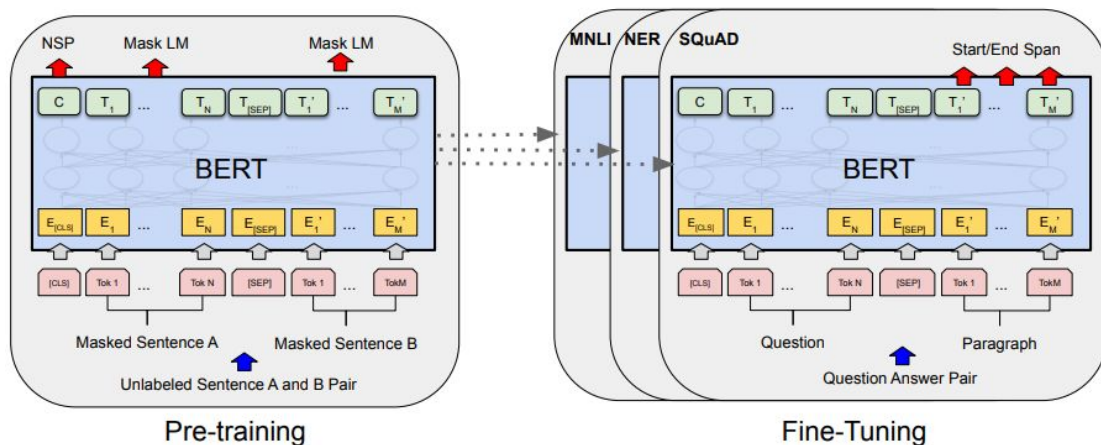
Transformers: Word Embedding

- For each word, we can convert them into a one-hot vector.
- We use the embedding layer to encode these one-hot vectors, which acts like a trainable lookup table.
- Dictionary: {are, is, machine, good, awesome, learning, love,}



Case Study: BERT

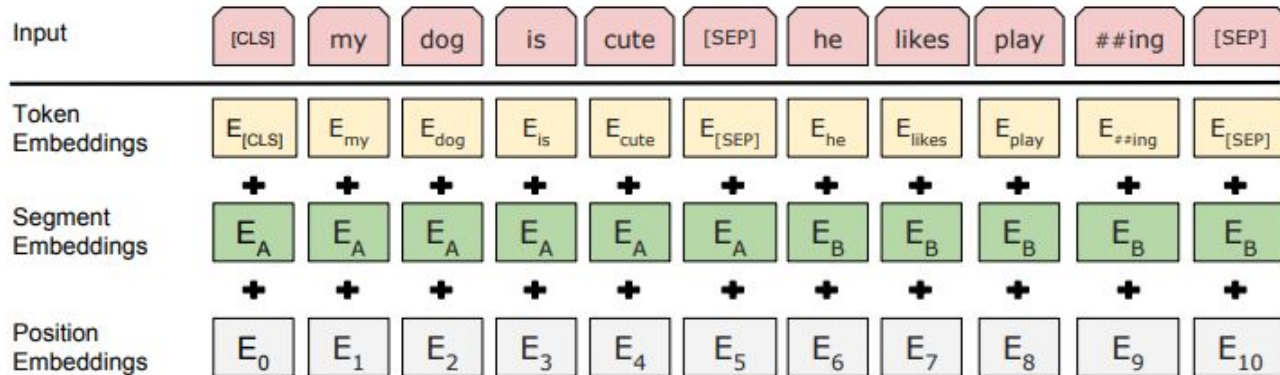
- Bidirectional Encoder Representations from Transformers.
- BERT is designed to understand the text by considering both the words before and after it.
- BERT consists of transformer encoders and takes the entire sentence as the input.
- The pre-trained BERT model can be finetuned with just one additional output layer to create state-of-the-art models for a wide range of tasks.



Devlin, Jacob. "Bert: Pre-training of deep bidirectional transformers for language understanding." *arXiv preprint arXiv:1810.04805* (2018).

BERT

- A [CLS] token is inserted at the start of every sequence, and the two sentences in the sequence are separated by a [SEP] token.
- The final hidden state corresponding to this token is used as the aggregate sequence representation for classification tasks.
- In addition to the positional information, BERT contains a segment embeddings to differentiate the sentences.

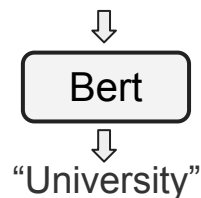


BERT Pretraining

- BERT is pretrained using two unsupervised tasks:
 - Masked Language Modeling (MLM)
 - We simply mask some percentage of the input tokens at random, and then predict those masked tokens.
 - Next Sentence Prediction (NSP)
 - Given two sentences, A and B, predict whether B is A's following sentence.

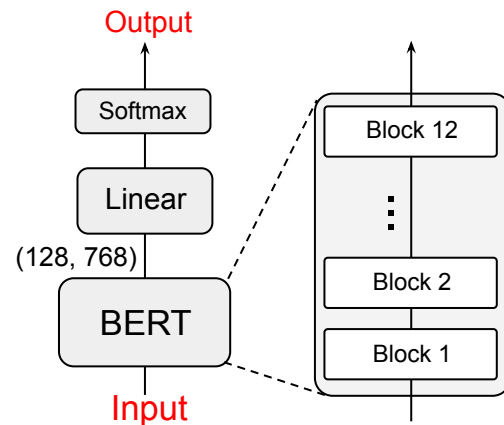
“New York University is a great school.”

“New York **University** is a great school.”

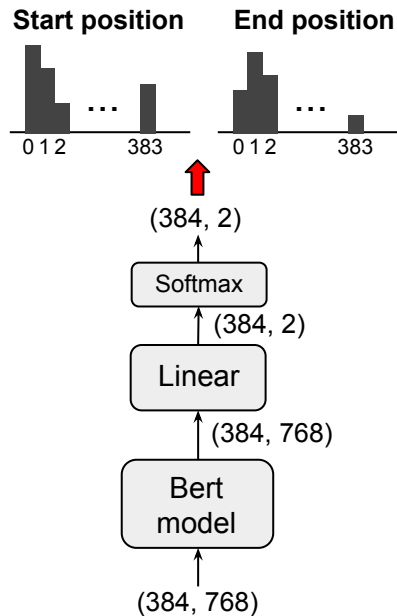


Downstream Tasks

- For text classification task, Bert will return a binary output.
 - Single sentence task (SST-2): The task is to predict the sentiment of a given sentence.
- The input may contain a single sentence, or a pair of sentences.
 - Similarity and Paraphrase tasks (MRPC): Is the second sentence a paraphrase of the first sentence.



Downstream Tasks



Context paragraph

“Similarly, movies and television often revert to standard, clichéd snatches of **classical music** to convey refinement or opulence: some of the most-often heard pieces in this category include Bach’s Cello Suite No. 1, Mozart’s Eine kleine Nachtmusik, Vivaldi’s Four Seasons, Mussorgsky’s Night on Bald Mountain (as orchestrated by Rimsky-Korsakov), and Rossini’s William Tell Overture.”

Question

“Who wrote William Tell Overture?”

Answer

Classical_music (12, 13)

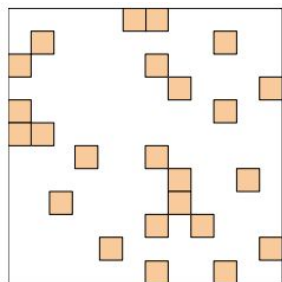
- In Question Answering tasks, an input sample consists of a context paragraph and a question with a total length of 384.
- The goal is to find, for each question, a span of text in the context paragraph that answers that question.
- DNN model produces the answers by generating the start and end positions of the text span.

BERT Performance

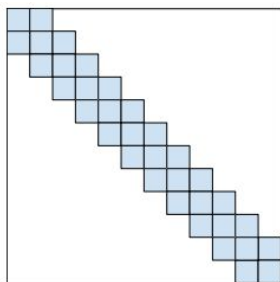
System	MNLI-(m/mm) 392k	QQP 363k	QNLI 108k	SST-2 67k	CoLA 8.5k	STS-B 5.7k	MRPC 3.5k	RTE 2.5k	Average
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
BERT _{BASE}	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
BERT _{LARGE}	86.7/85.9	72.1	92.7	94.9	60.5	86.5	89.3	70.1	82.1

- BERT can achieve better performance over GLUE datasets than GPT-1.

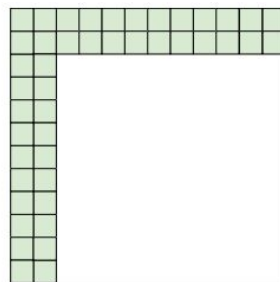
Efficient Self-Attention Design



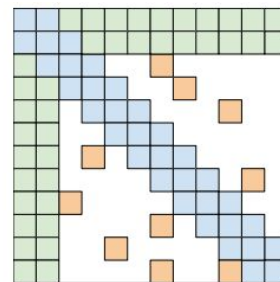
(a) Random attention



(b) Window attention

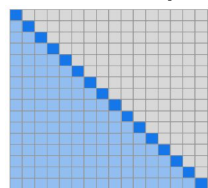


(c) Global Attention

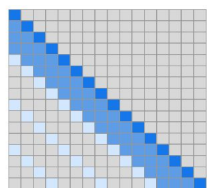


(d) BIGBIRD

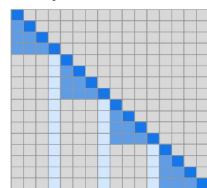
Sparse Transformer (2019)



Original

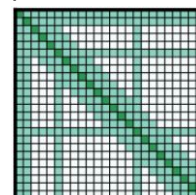
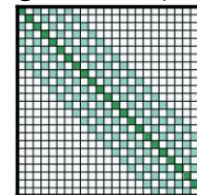
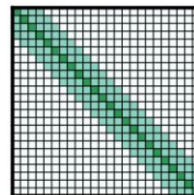


Strided

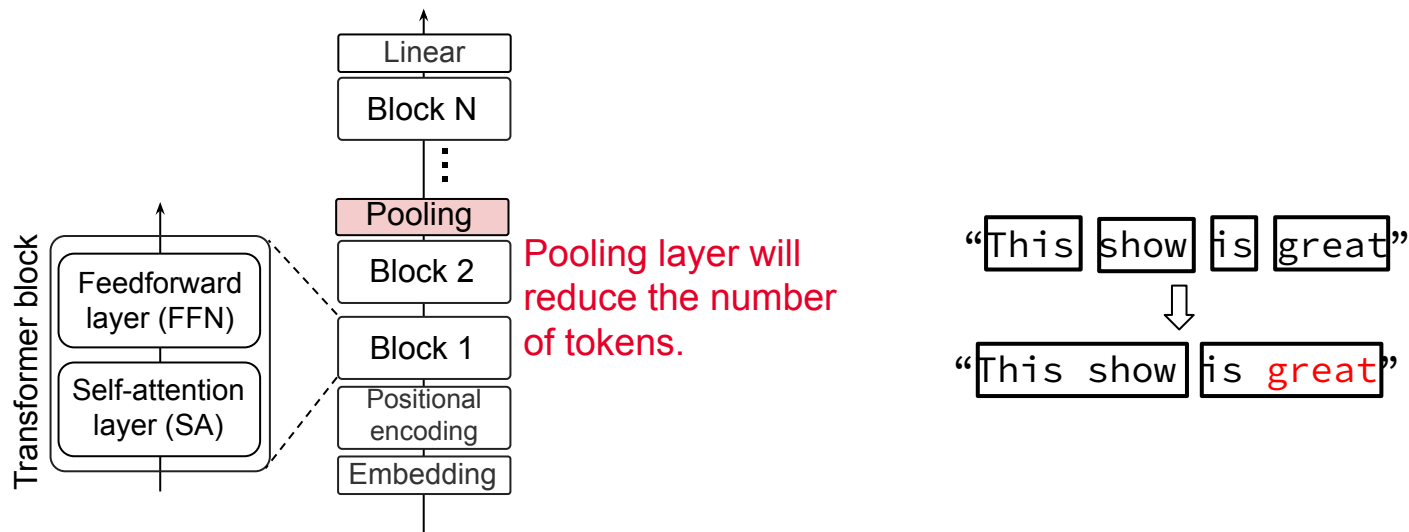


Fixed

Longformer (2020)

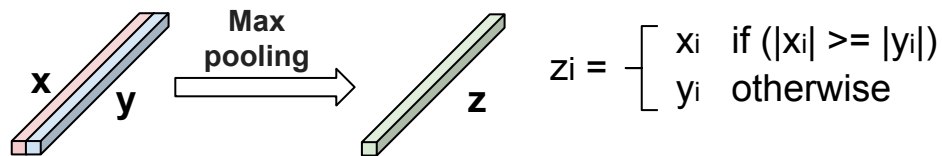


Token Merging

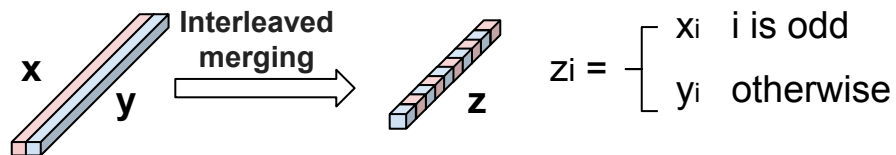
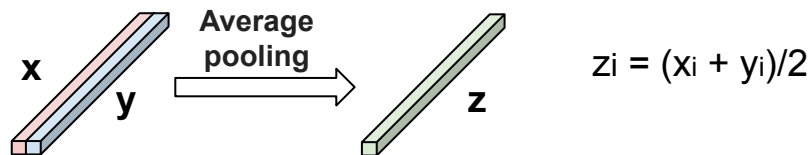


- We can reduce the number of tokens by merging them together.

Token Merging



- x, y are two token vectors with length of E

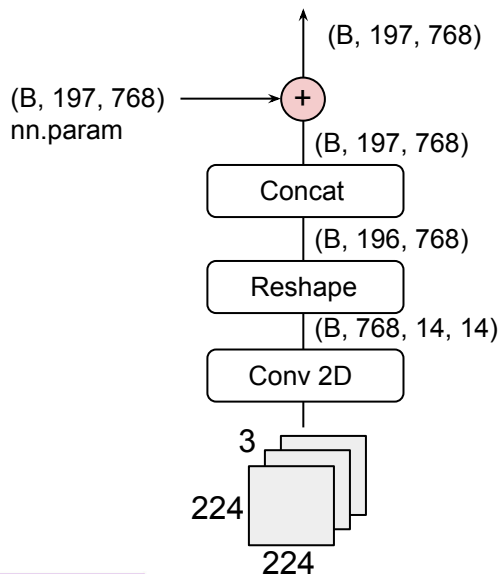


Topics

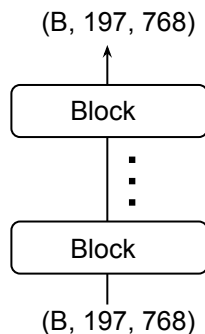
- Transformer basics
- Vision transformer
- AIGC
 - LLM
 - Diffusion model
- Self-supervised learning

Vision Transformer

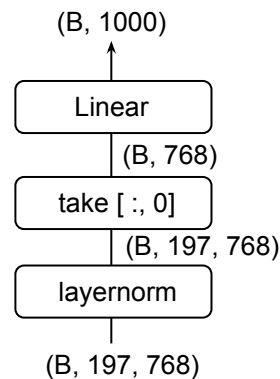
- Transformer architecture can also be applied over the computer vision tasks.



(part 1)



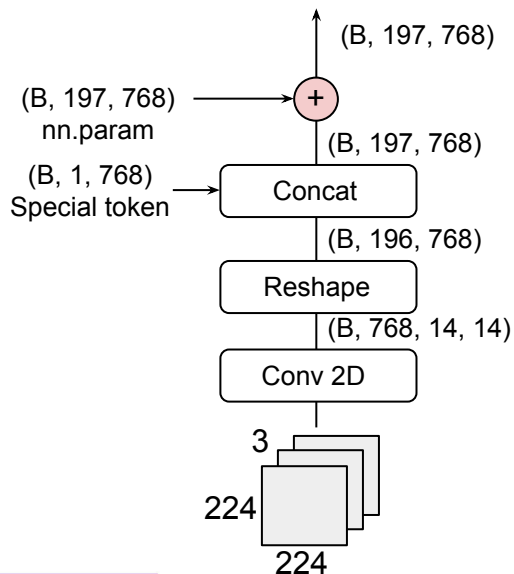
(part 2)



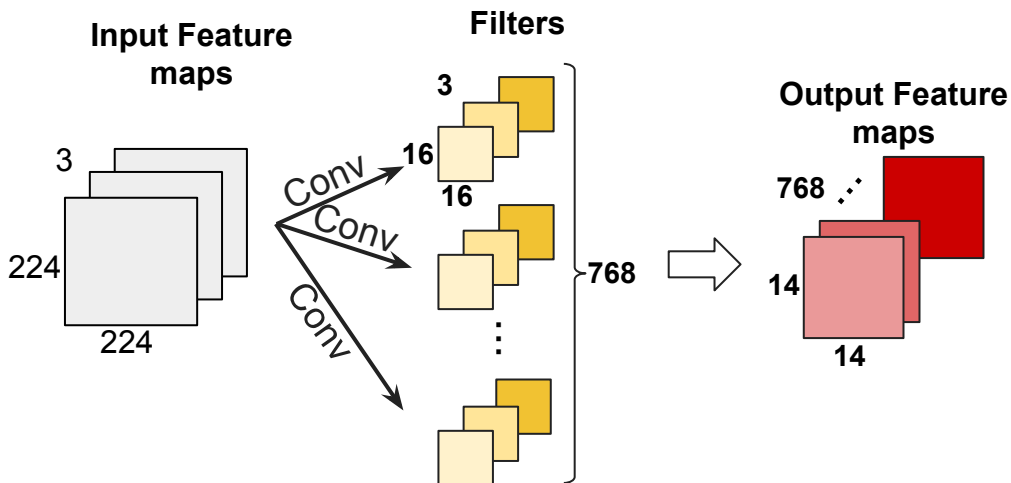
(part 3)

Vision Transformer

- Transformer architecture can also be applied over the computer vision tasks.



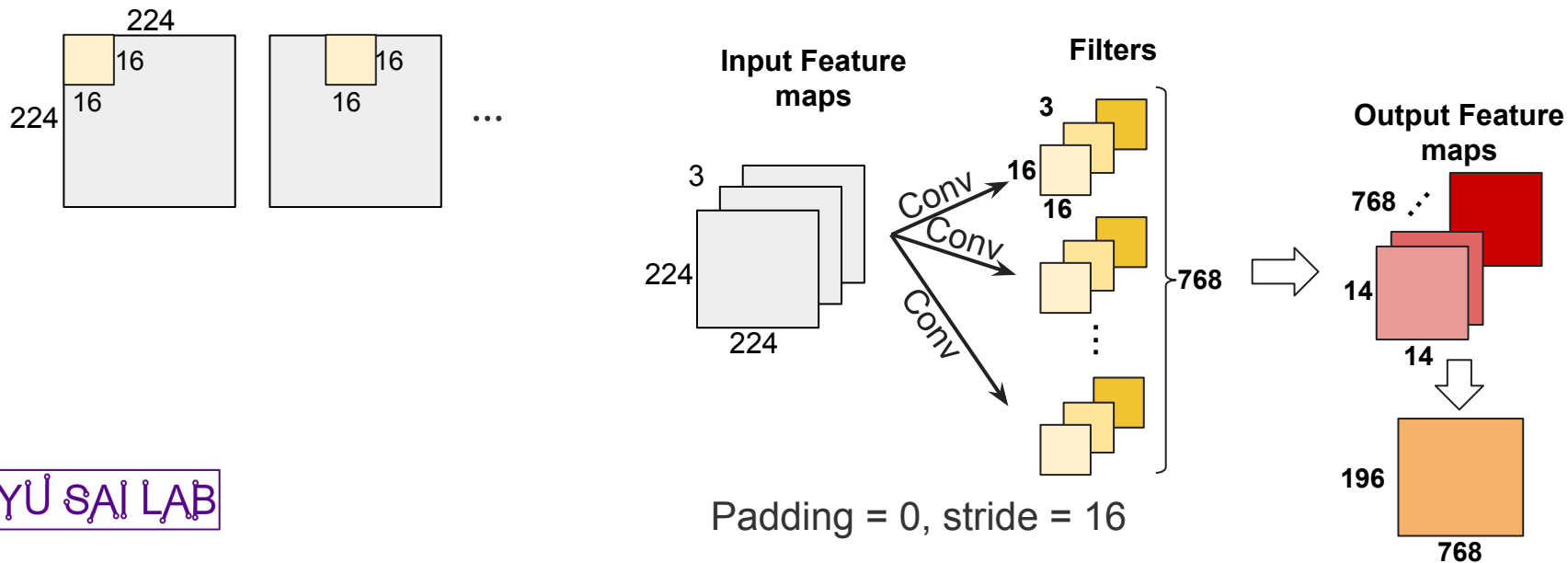
(part 1)



Padding = 0, stride = 16

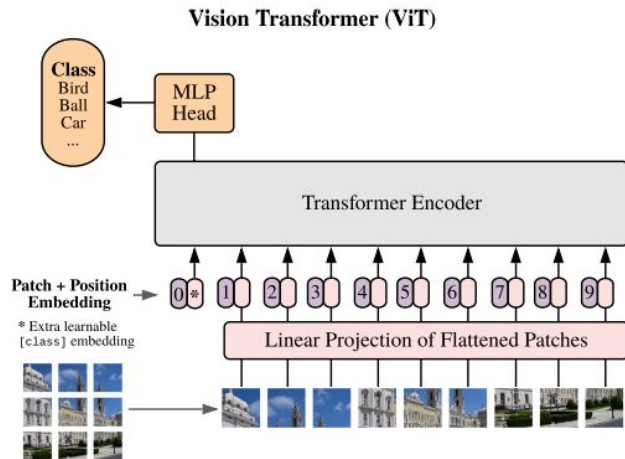
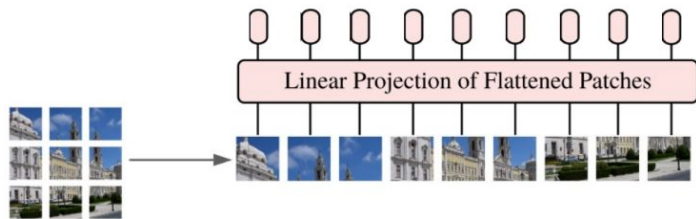
Vision Transformer

- Transformer architecture can also be applied over the computer vision tasks.



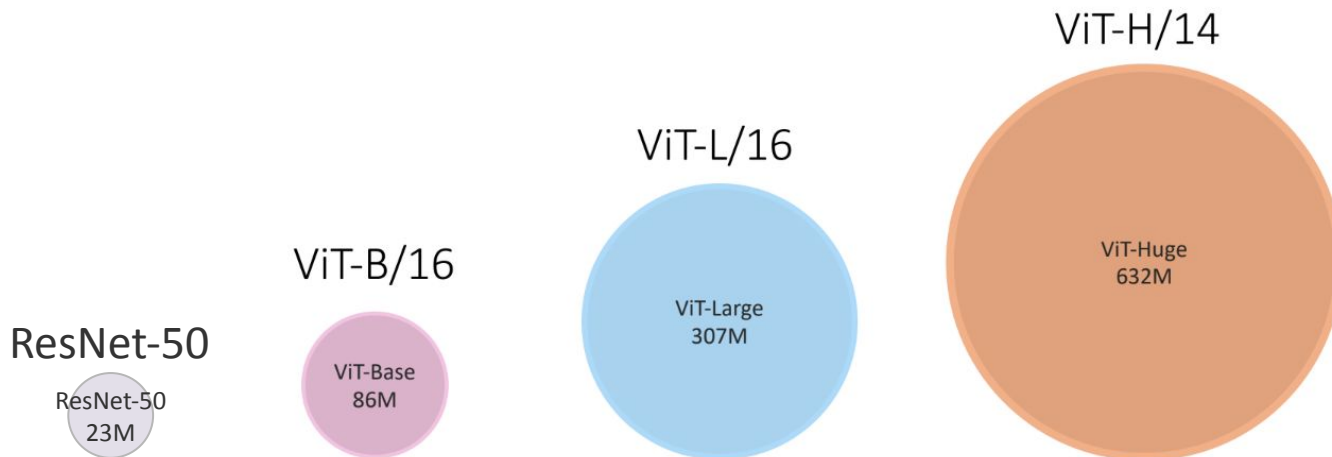
Vision Transformer

- An image $C \times H \times W$ is divided into patches of $C \times P \times P$. P is 16×16 in the previous example.
- They are then flattened and linearly projected to E (e.g., 768) dimensions for a sequence of $(H/P) \times (W/P)$ tokens.

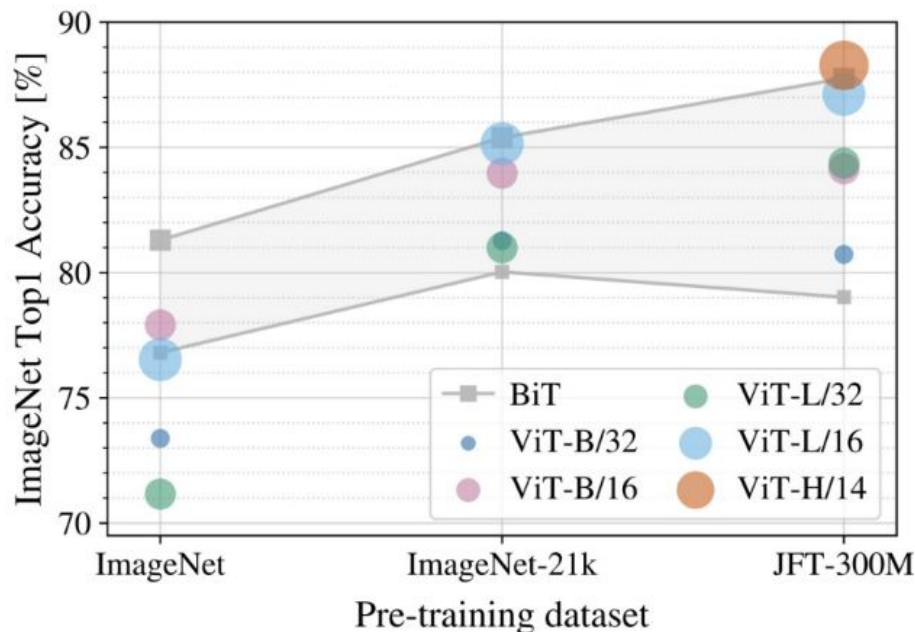


- A classification [CLS] token is inserted at the start of the tokens.

Vision Transformer



Vision Transformer

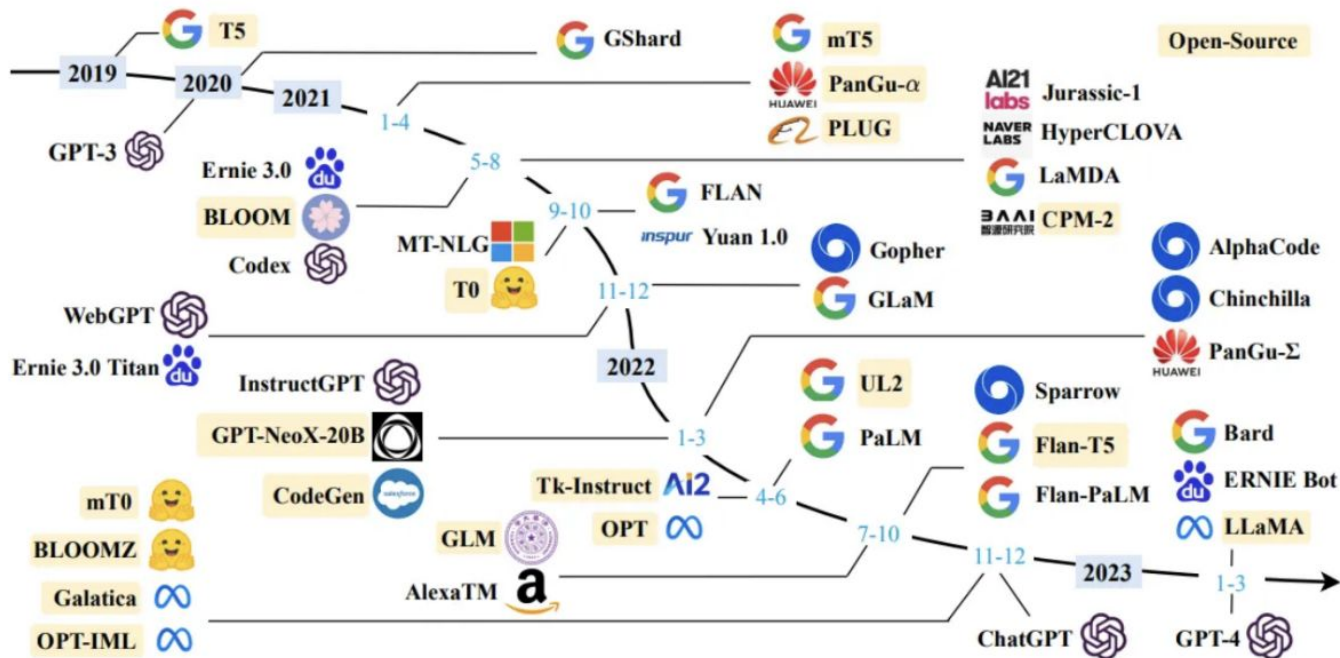


- Accuracy increases as the training dataset grow.
- ResNet 50 can achieves an accuracy between 75-80% on ImageNet.
- ViT does not strike an efficient balance between parameter count and accuracy.

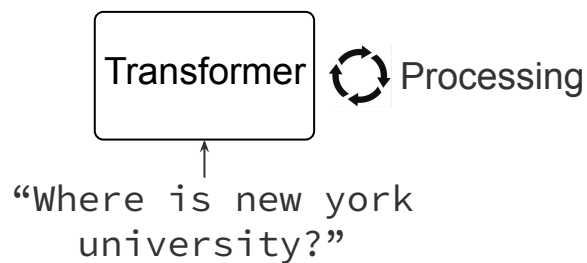
Topics

- Transformer basics
- Vision transformer
- AIGC
 - LLM
 - Diffusion model
- Self-supervised learning

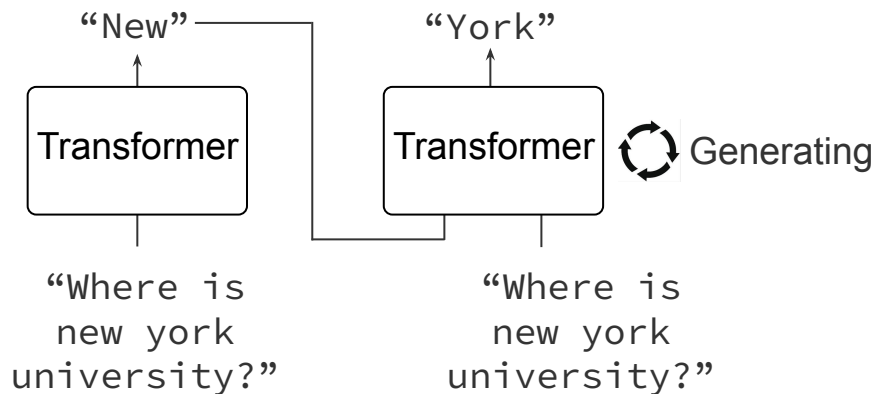
Large Language Models (LLMs)



Transformers as a Generative AI Tool

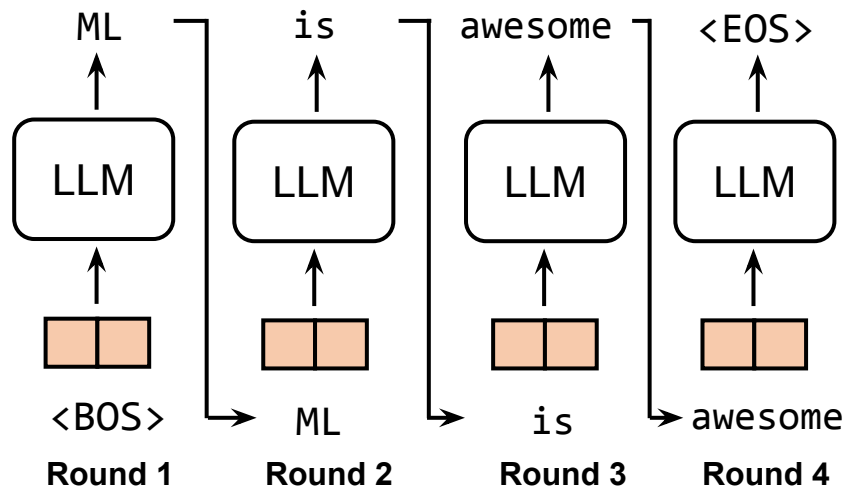
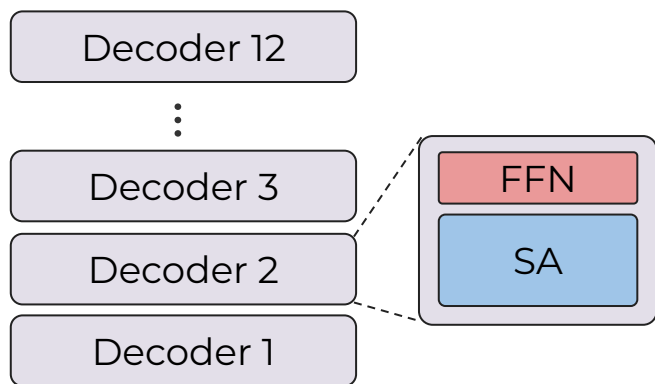


Step 1



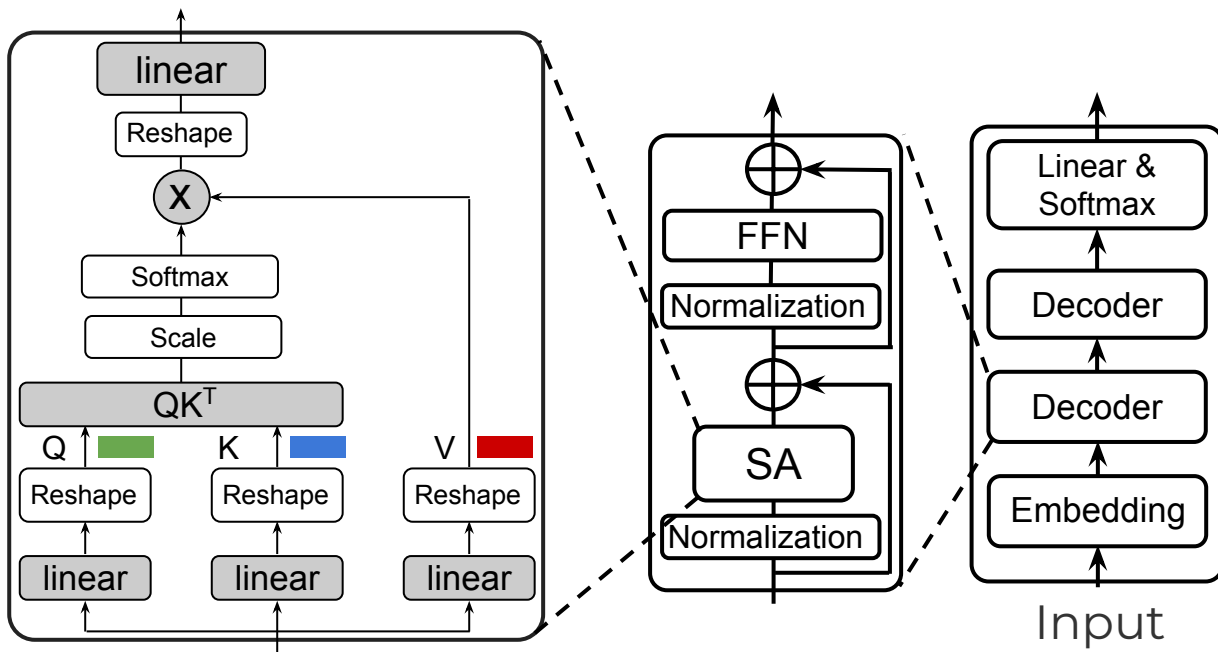
Step 2

Transformers as a Generative AI Tool



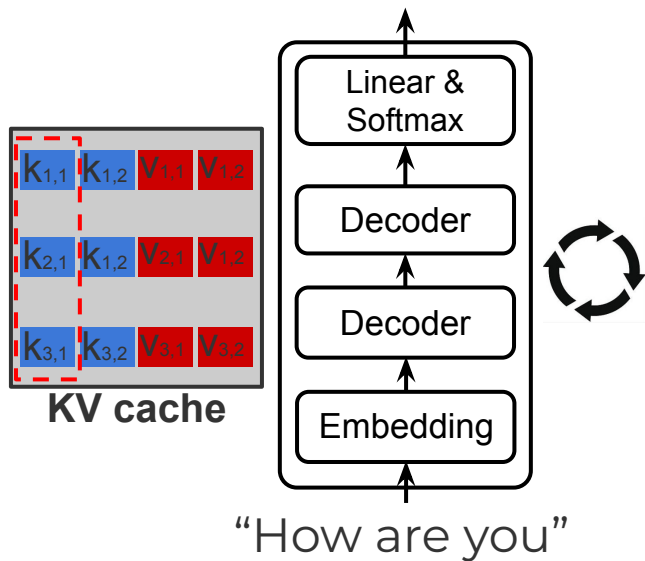
- Each token is generated in an autoregressive manner.

Transformers as a Generative AI Tool



- We need to buffer the v and k for later usage.

GPT-2: Prefilling

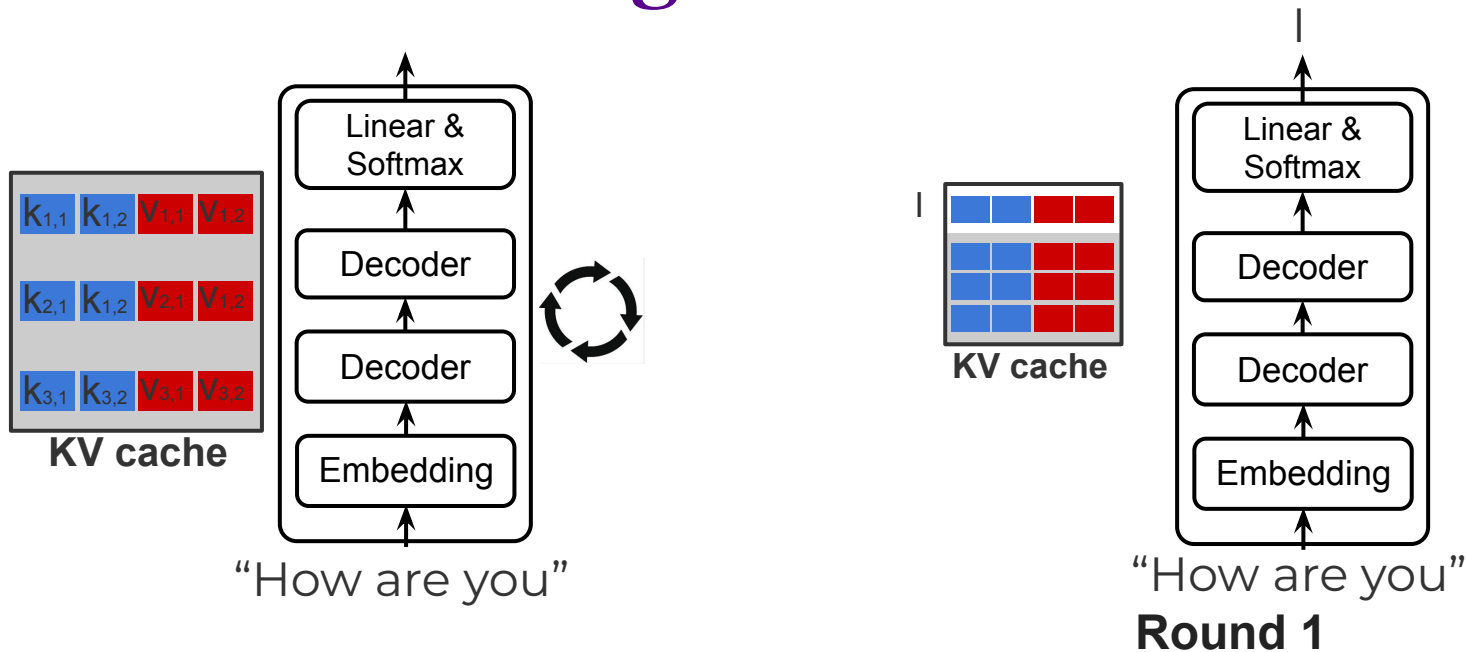


$k_{i,j}$ Key vector for i th token in j th layer
($1 \times E$)

$v_{i,j}$ Value vector for i th token in j th layer
($1 \times E$)

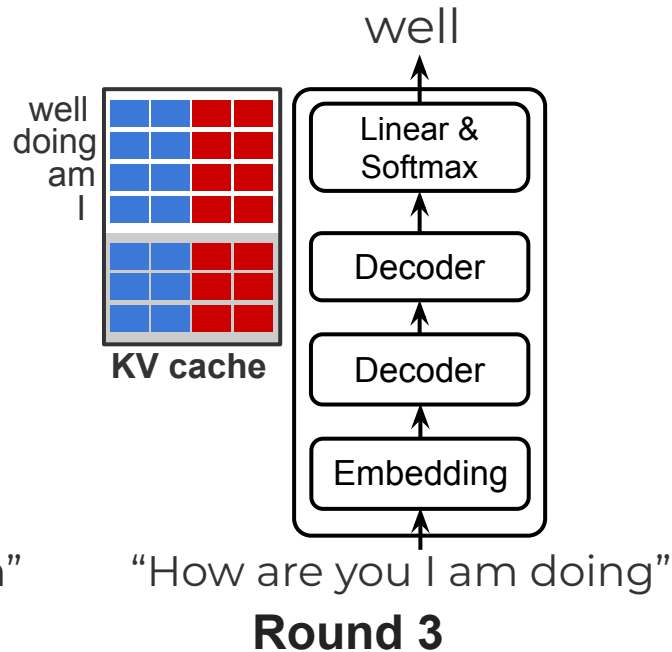
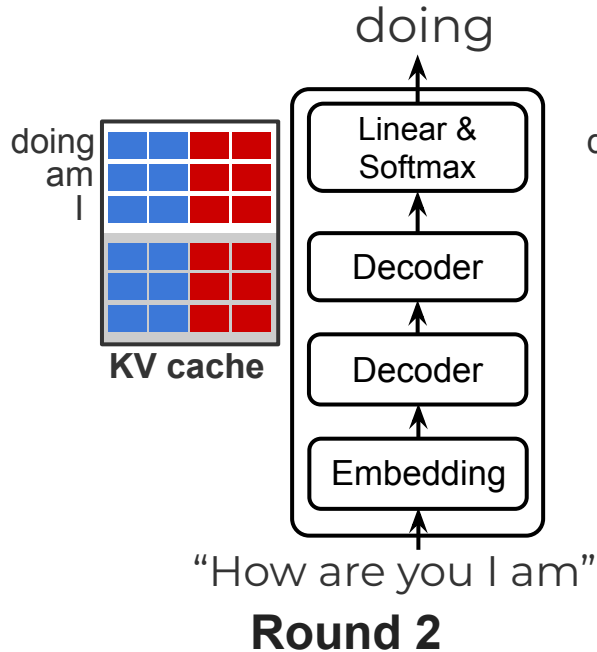
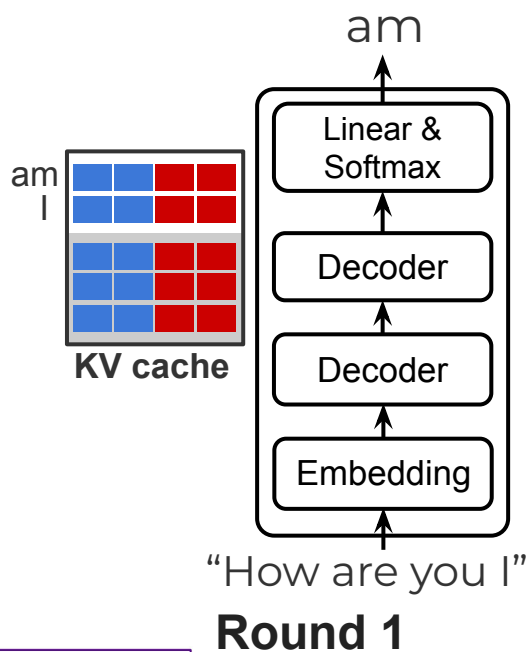
- During the prefilling stage, LLM processes the entire prompt, or context tokens jointly, saving the KV vectors into the memory.

GPT-2: Decoding

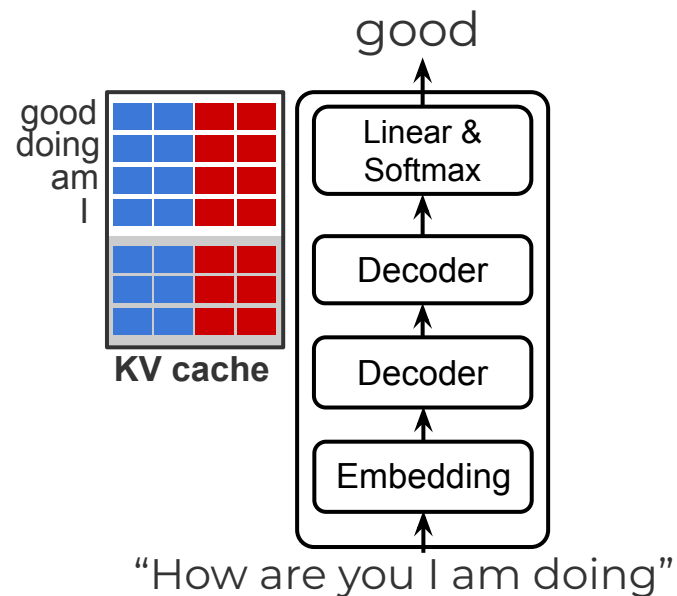
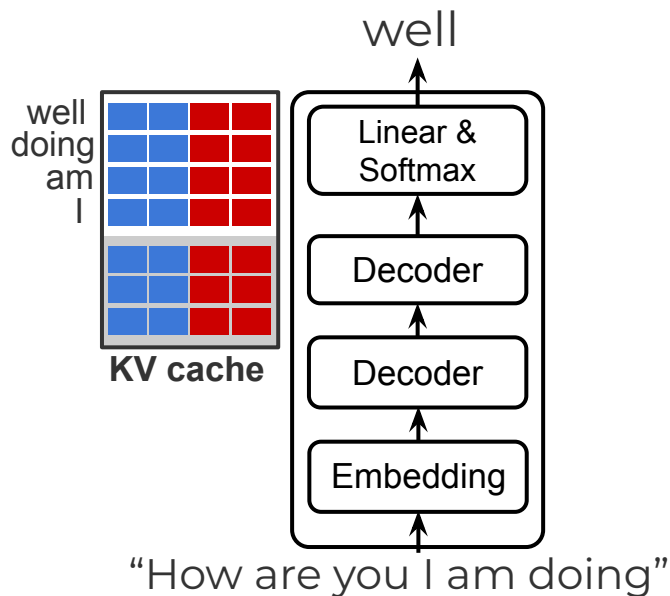


- During the decoding stage, LLM generates the responses in an autoregressive way.

GPT-2: Decoding

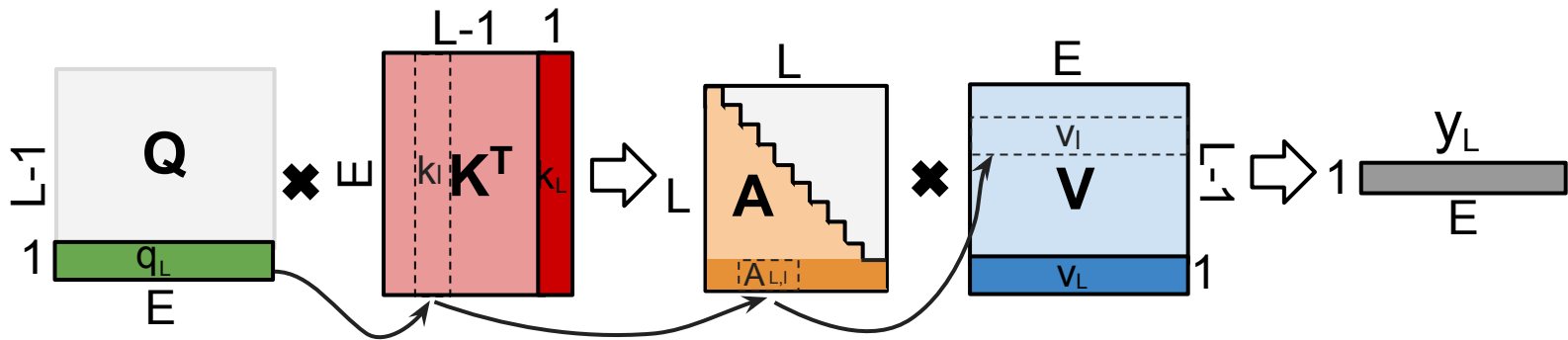


GPT-2: Decoding



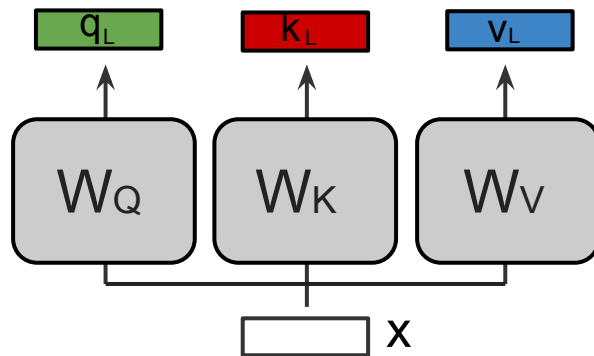
- We can simply select the token with the highest score. But better results are achieved if the model considers other words as well. So a better strategy is to sample a word from the entire list using the score as the probability of selecting that word.

Why KV Cache Saves Computation?



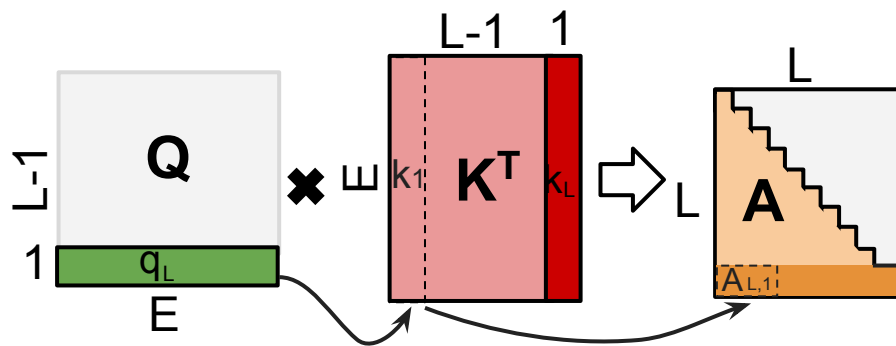
- During the decoding phase, new tokens are continuously generated and must be processed using the buffered K and V vectors to generate subsequent tokens.
- Without a KV cache, all previous K and V vectors must be recomputed, resulting in significant computational overhead.

Why KV Cache Saves Computation?



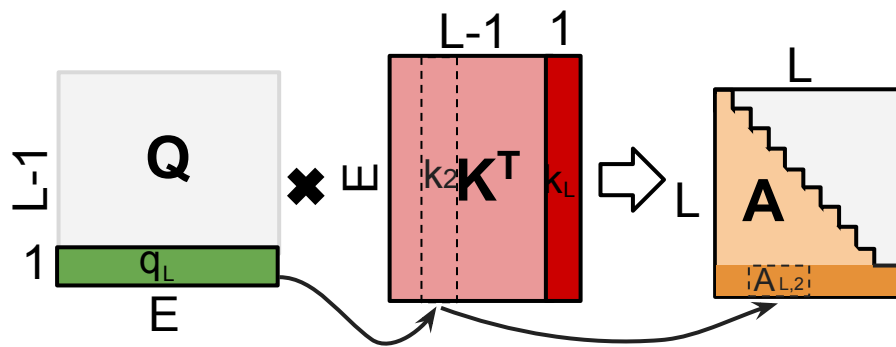
- Given the input, the q_L , k_L , v_L are first computed by passing through the linear layers.
- After that, the k_l , v_l vectors ($l=1, \dots, L-1$) are also loaded from the memory.

Why KV Cache Saves Computation?



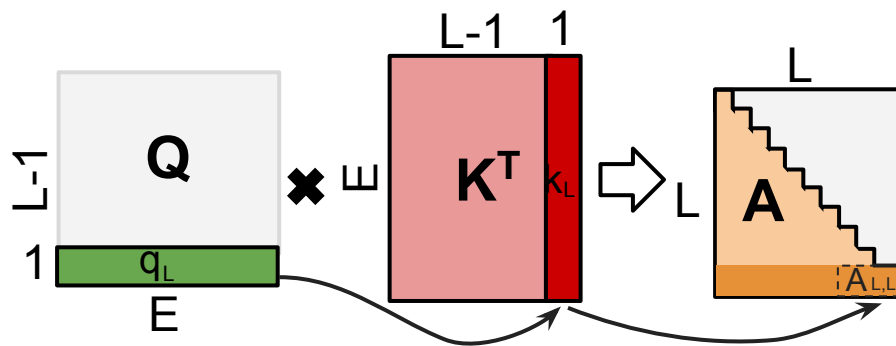
- K and V are loaded from the memory, the q vector of the current token (q_L) is multiplied with the each of the key vector k_i , ($i=1 \dots L$) to produce the result $A_{L,i}$

Why KV Cache Saves Computation?



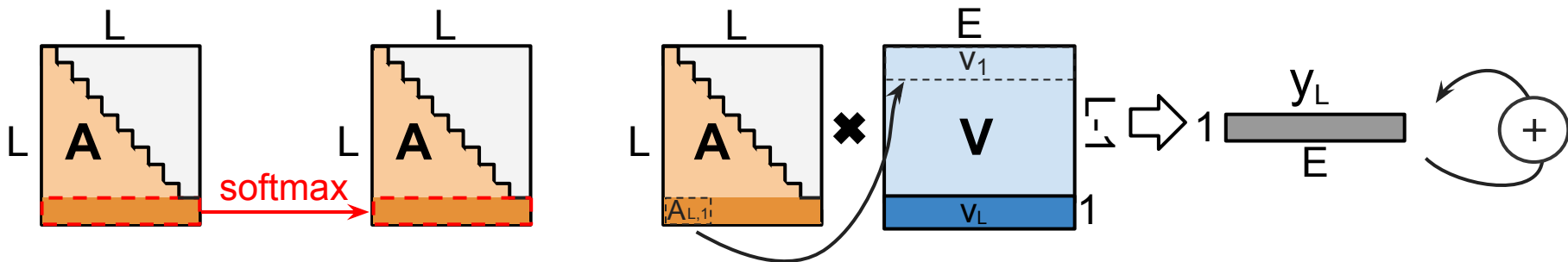
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Why KV Cache Saves Computation?



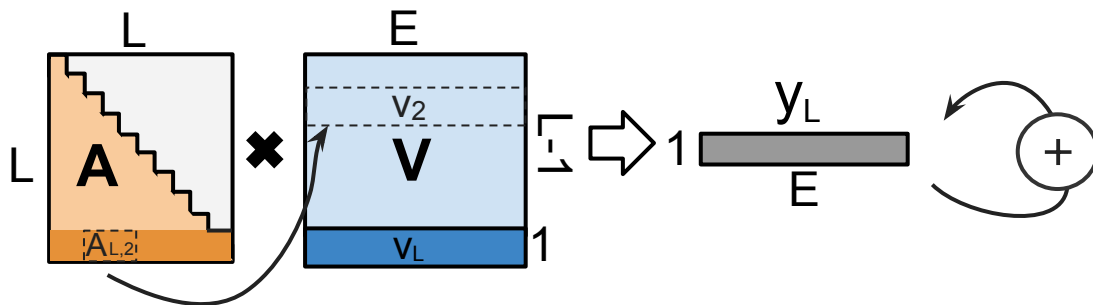
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Why KV Cache Saves Computation?



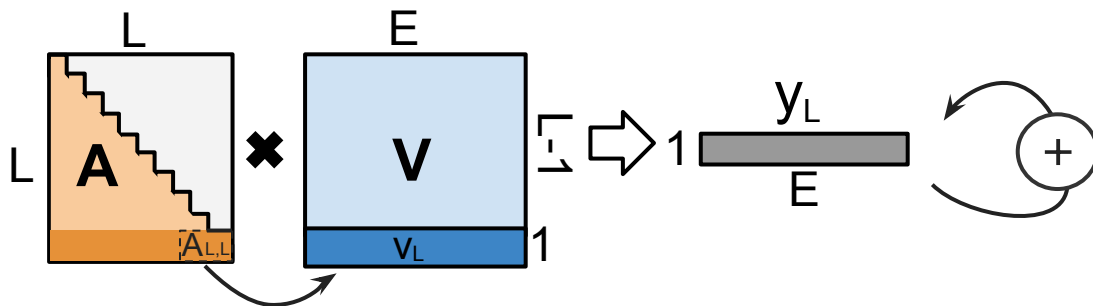
- Afterwards, the computed $A_{L,i}$ ($i=1 \dots L$) will then passed to softmax function.
- Then each element of A_L will then multiplied with v_i ($i=1 \dots L$) and elementwise sum together.

Why KV Cache Saves Computation?



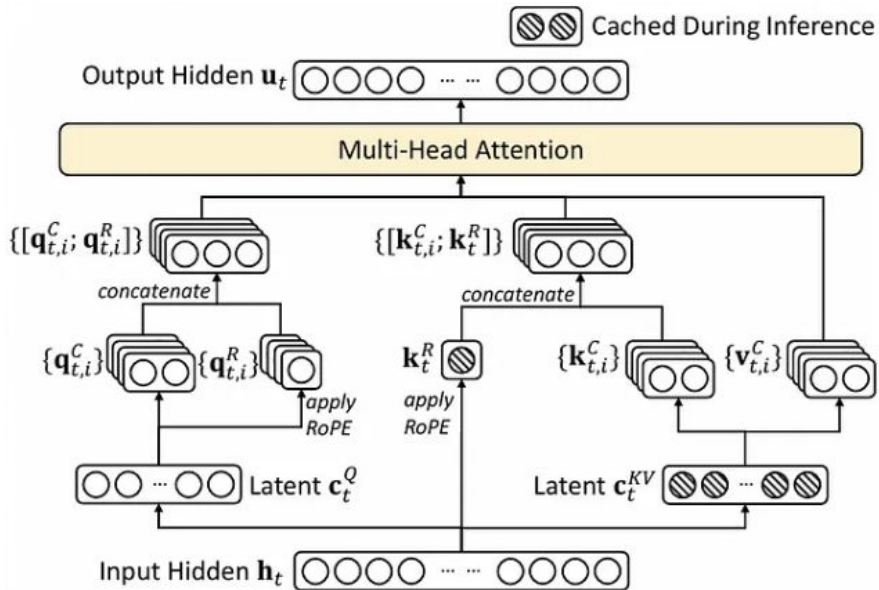
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Why KV Cache Saves Computation?



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Deepseek V3



$$\mathbf{c}_t^Q = W^{DQ} \mathbf{h}_t, \quad (37)$$

$$[\mathbf{q}_{t,1}^C; \mathbf{q}_{t,2}^C; \dots; \mathbf{q}_{t,n_h}^C] = \mathbf{q}_t^C = W^{UQ} \mathbf{c}_t^Q, \quad (38)$$

$$[\mathbf{q}_{t,1}^R; \mathbf{q}_{t,2}^R; \dots; \mathbf{q}_{t,n_h}^R] = \mathbf{q}_t^R = \text{RoPE}(W^{QR} \mathbf{c}_t^Q), \quad (39)$$

$$\mathbf{q}_{t,i} = [\mathbf{q}_{t,i}^C; \mathbf{q}_{t,i}^R], \quad (40)$$

$$\mathbf{c}_t^{KV} = W^{DKV} \mathbf{h}_t, \quad (41)$$

$$[\mathbf{k}_{t,1}^C; \mathbf{k}_{t,2}^C; \dots; \mathbf{k}_{t,n_h}^C] = \mathbf{k}_t^C = W^{UK} \mathbf{c}_t^{KV}, \quad (42)$$

$$\mathbf{k}_t^R = \text{RoPE}(W^{KR} \mathbf{h}_t), \quad (43)$$

$$\mathbf{k}_{t,i} = [\mathbf{k}_{t,i}^C; \mathbf{k}_t^R], \quad (44)$$

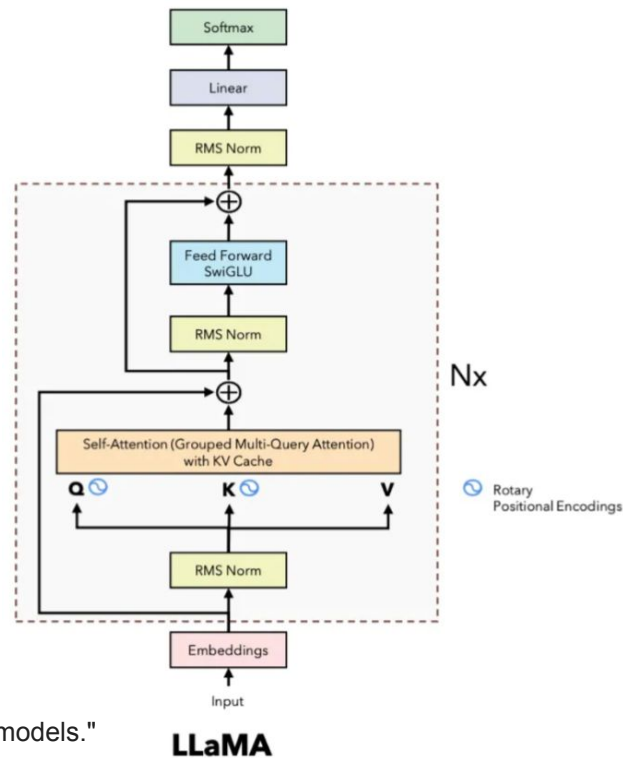
$$[\mathbf{v}_{t,1}^C; \mathbf{v}_{t,2}^C; \dots; \mathbf{v}_{t,n_h}^C] = \mathbf{v}_t^C = W^{UV} \mathbf{c}_t^{KV}, \quad (45)$$

$$\mathbf{o}_{t,i} = \sum_{j=1}^t \text{Softmax}_j \left(\frac{\mathbf{q}_{t,i}^T \mathbf{k}_{j,i}}{\sqrt{d_h + d_h^R}} \right) \mathbf{v}_{j,i}^C, \quad (46)$$

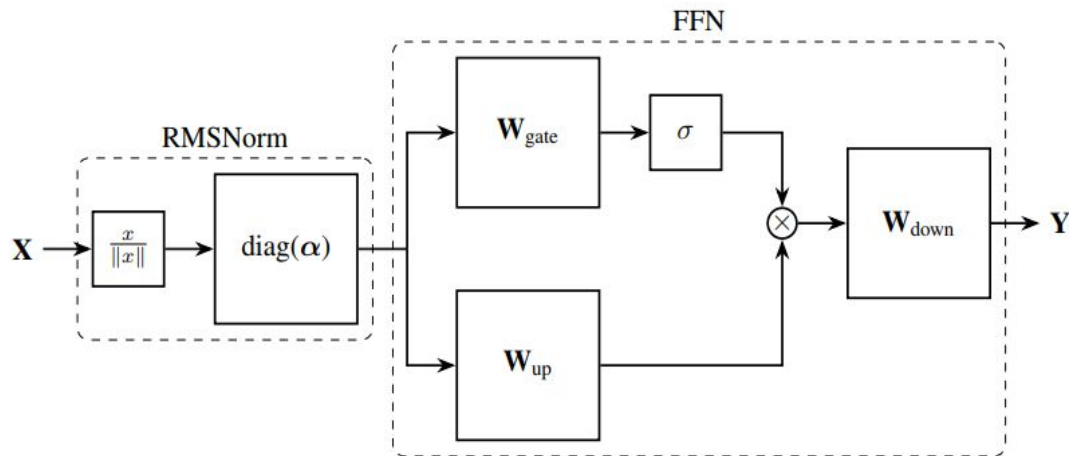
$$\mathbf{u}_t = W^O [\mathbf{o}_{t,1}; \mathbf{o}_{t,2}; \dots; \mathbf{o}_{t,n_h}], \quad (47)$$

LLaMA

- LLaMA has a similar architecture as GPT-2, with some minor differences:
 - RMSNorm is used to replace LayerNorm
 - SwiGLU
 - MLPs with gating



MLPs with Gating



- A lot of LLM models applies gated feed-forward network to replace the conventional FFN in the transformer.

How LLM is Trained?

- The loss function consists of two parts:

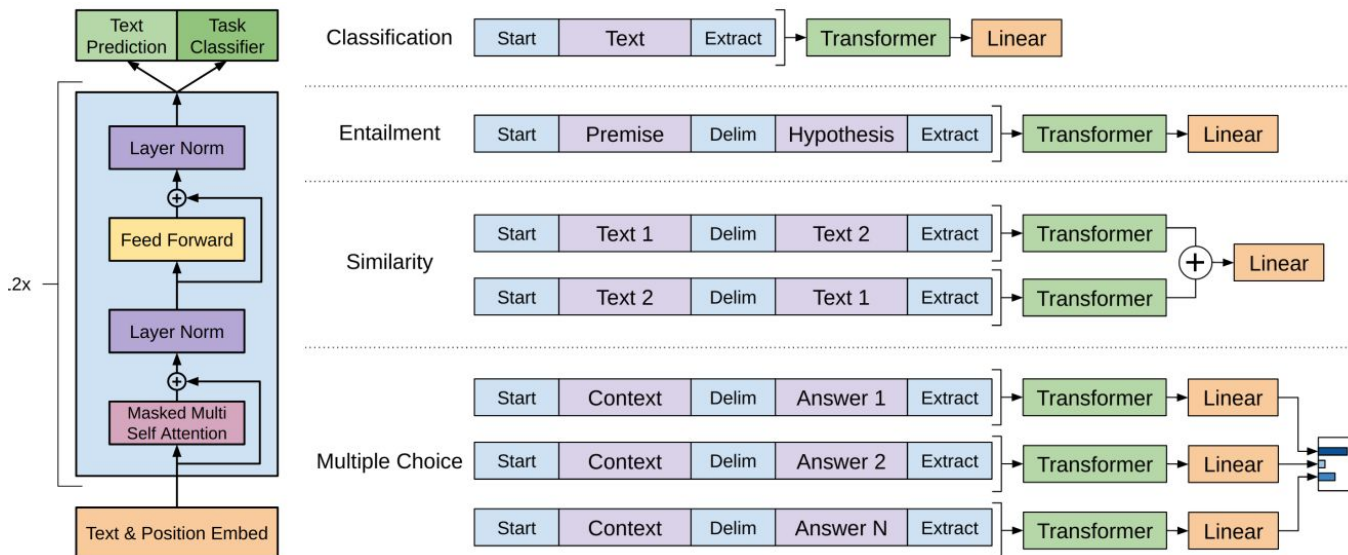
$$L_1(\mathcal{U}) = \sum \log P(u_i | u_{i-k}, \dots, u_{i-1}; \Theta)$$

“A newspaper article should contain these five main components: a headline, a byline, a lead/lede paragraph, an explanation, and any other additional information.”

A newspaper article should contain these five main **xxx** → “**components**” (GPT)

A newspaper article should **xxx** these five main components: a headline, a byline, a lead/lede paragraph, an explanation, and any other additional information. → “**contain**” (BERT)

How LLM is Trained?



$$L_3(\mathcal{C}) = L_2(\mathcal{C}) + \lambda * L_1(\mathcal{C})$$

Presentations

- [Longformer: The Long-Document Transformer](#) (Aadi)
- [Language Models are Unsupervised Multitask Learners](#) (Riya)
- [LLaMA: Open and Efficient Foundation Language Models](#) (Greeshma)

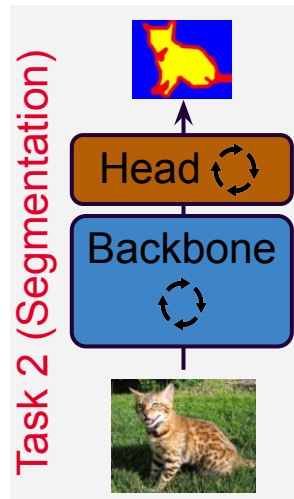
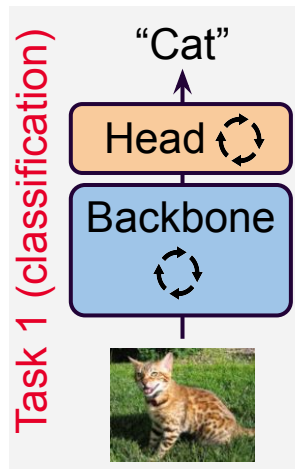
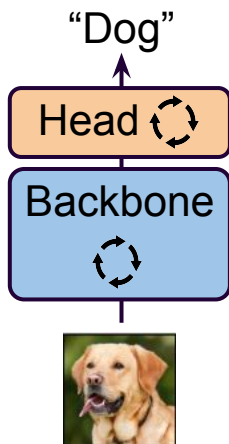
Topics

- Transformer basics
- Vision transformer
- AIGC
 - LLM
 - Diffusion model
- Self-supervised learning

Self-Supervised Learning

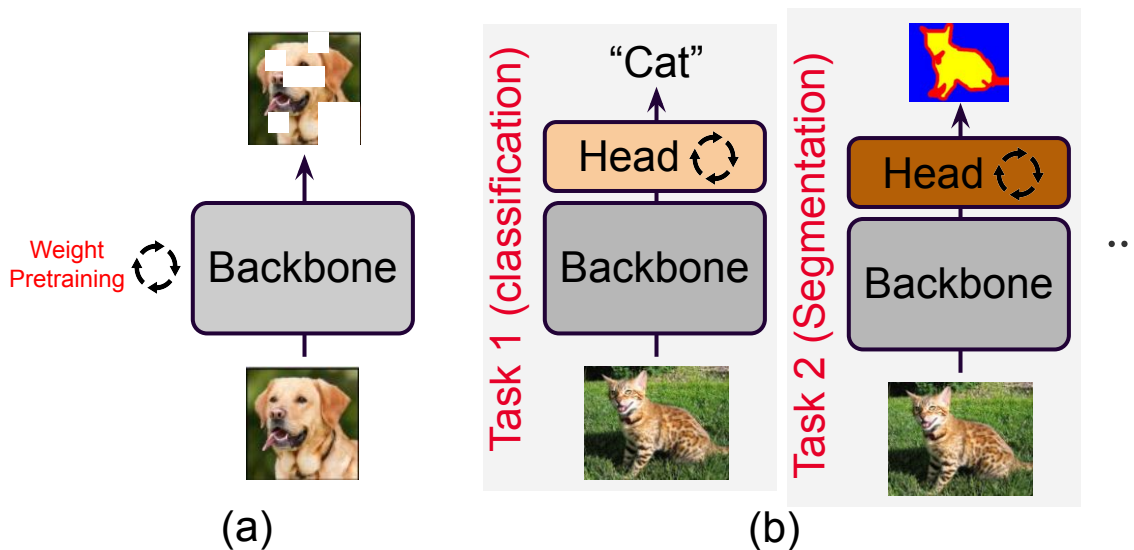
- Self-Supervised Learning (SSL) is a paradigm that leverages intrinsic structures within unlabeled data to create pretext tasks, enabling models to learn meaningful representations that can be fine-tuned for downstream applications.

Weight update 



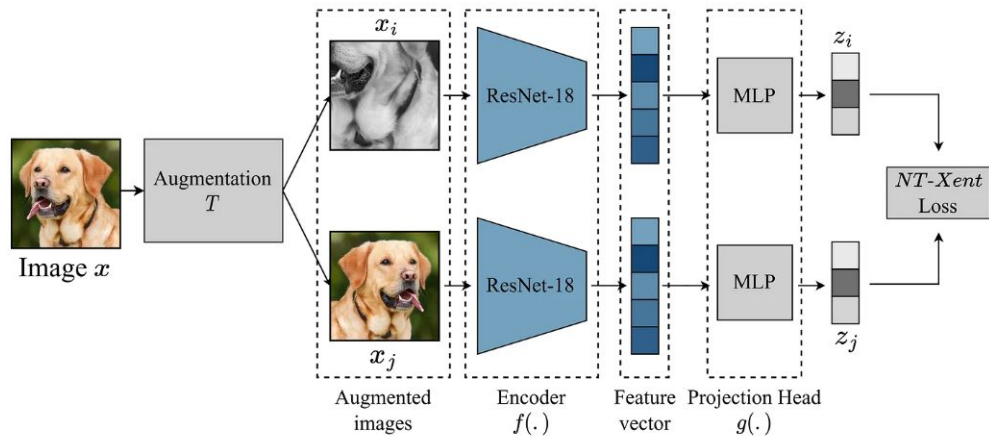
Self-Supervised Learning

- Self-Supervised Learning (SSL) is a paradigm that leverages intrinsic structures within unlabeled data to create pretext tasks, enabling models to learn meaningful representations that can be fine-tuned for downstream applications.



Popular SSL Methods: Contrastive Learning

- Contrastive Learning is a framework in which models learn meaningful representations by contrasting positive pairs (similar data points) with negative pairs (dissimilar data points), encouraging the embedding space to capture semantic similarities and differences.

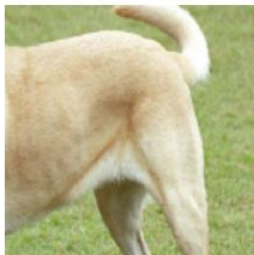


SimCLR framework. Image by author.

Popular SSL Methods: Contrastive Learning



(a) Original



(b) Crop and resize



(c) Crop, resize (and flip)



(d) Color distort. (drop)



(e) Color distort. (jitter)



(f) Rotate $\{90^\circ, 180^\circ, 270^\circ\}$



(g) Cutout



(h) Gaussian noise



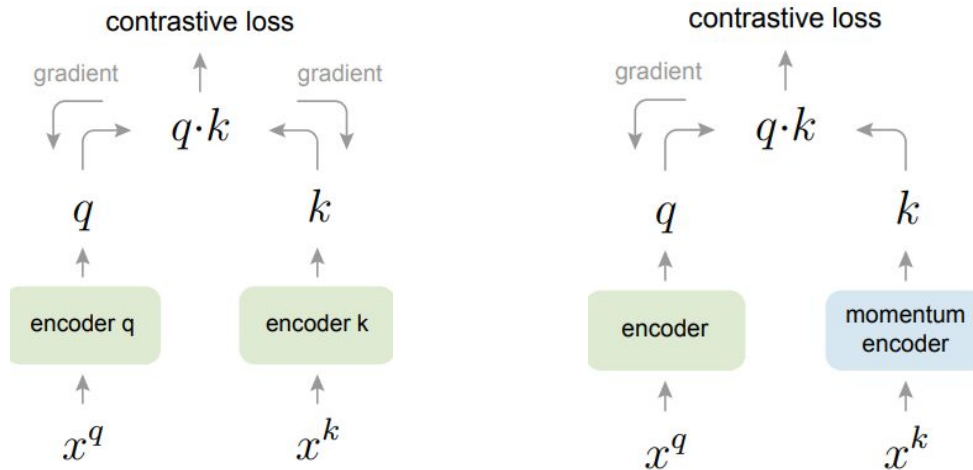
(i) Gaussian blur



(j) Sobel filtering

- The current augmentation approaches adopted by the AI community including random crop (with flip and resize), color distortion, and Gaussian blur.

Momentum Contrast SSL (MoCo)



- In the training process, only query encoder is updated, momentum encoder doesn't change.

$$\theta_k \leftarrow m\theta_k + (1 - m)\theta_q.$$

- Only the encoder is updated.

Knowledge Distillation with No Labels (DINO)

Algorithm 1 DINO PyTorch pseudocode w/o multi-crop.

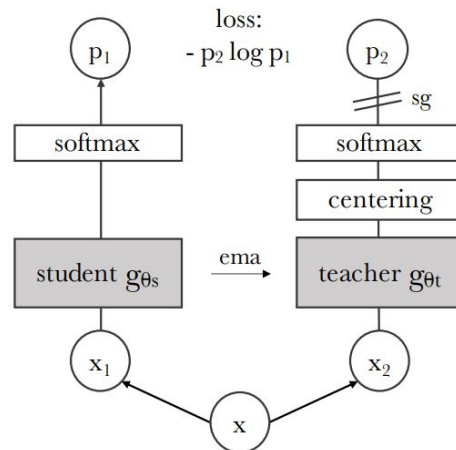
```
# gs, gt: student and teacher networks
# C: center (K)
# tps, tpt: student and teacher temperatures
# l, m: network and center momentum rates
gt.params = gs.params
for x in loader: # load a minibatch x with n samples
    x1, x2 = augment(x), augment(x) # random views

    s1, s2 = gs(x1), gs(x2) # student output n-by-K
    t1, t2 = gt(x1), gt(x2) # teacher output n-by-K

    loss = H(t1, s2)/2 + H(t2, s1)/2
    loss.backward() # back-propagate

    # student, teacher and center updates
    update(gs) # SGD
    gt.params = l*gt.params + (1-l)*gs.params
    C = m*C + (1-m)*cat([t1, t2]).mean(dim=0)

def H(t, s):
    t = t.detach() # stop gradient
    s = softmax(s / tps, dim=1)
    t = softmax((t - C) / tpt, dim=1) # center + sharpen
    return - (t * log(s)).sum(dim=1).mean()
```

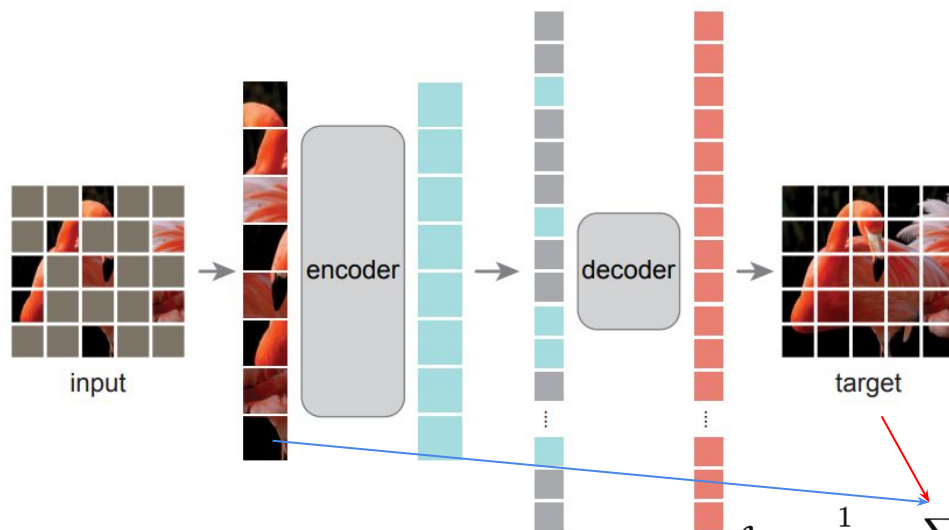


DINO (2021)

- During the backpropagation, only the student DNN is updated.
- The teacher updates its weight periodically using the following formula:

$$gt.params = l*gt.params + (1-l)*gs.params$$

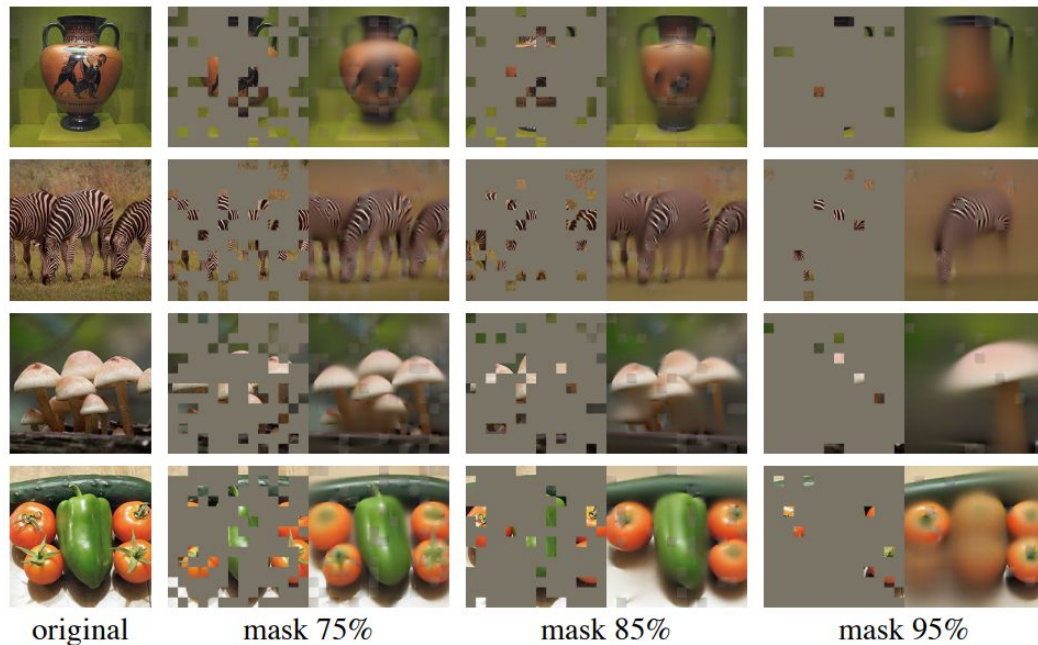
Masked AutoEncoder (MAE)



$$\mathcal{L} = \frac{1}{N_{\text{masked}}} \sum_{i \in \text{masked}} \|\hat{x}_i - x_i\|^2$$

- The input image is masked, the unmasked image patches will be sent to the encoder.
- The decoder will infer the masked portion of the image.

Self-Supervised Learning: Masked Autoencoder



JEPA

