

DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING



Language Model Architecture

COMP4901Y

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Overview



- What is a language model?
- Tokenization:
 - How do we represent language to machines?
- Model categorization:
 - Encoder-only, decoder-only, encoder-decoder.
- Training objectives:
 - How are large language models (LLM) trained?
- Transformer architecture:
 - The main innovation that enabled large language models.



Language Model





- The classic definition of a *language model (LM)* is a probability distribution over sequences of tokens.
- Suppose we have a vocabulary $\mathcal V$ of a set of tokens.
- A language model P assigns each sequence of tokens $x_1, x_2, ..., x_L \in \mathcal{V}$ to a probability (a number between 0 and 1): $p(x_1, x_2, ..., x_L) \in [0,1]$.
- The probability intuitively tells us how "good" a sequence of tokens is.
 - For example, if the vocabulary is $\mathcal{V} = \{\text{ate, ball, cheese, mouse, the}\}\$, the language model might assign:

```
p(\text{the, mouse, ate, the, cheese}) = 0.02

p(\text{the, cheese, ate, the, mouse}) = 0.01

p(\text{mouse, the, the, chesse, ate}) = 0.0001
```





- A language model *P* takes a sequence and returns a probability to assess its goodness.
- We can also generate a sequence given a language model.
- The purest way to do this is to sample a sequence $x_{1:L}$ from the language model P with probability equal to $p(x_{1:L})$ denoted:

$$x_{1:L} \sim P$$





• A common way to write the joint distribution $p(x_{1:L})$ of a sequence to $x_{1:L}$ is using the *chain rule of probablity*:

$$p(x_{1:L}) = p(x_1)p(x_2|x_1)p(x_3|x_1,x_2) \dots p(x_L|x_{1:L-1}) = \prod_{i=1}^{L} p(x_i|x_{1:i-1})$$

- In particular, $p(x_i|x_{1:i-1})$ is a conditional probability distribution of the next token x_i given the previous tokens $x_{1:i-1}$.
- An autoregressive language model is one where each conditional distribution $p(x_i|x_{1:i-1})$ can be computed efficiently (e.g., using a feedforward neural network).



Tokenization

Tokenization



• Recall: language model P is a probability distribution over a sequence of tokens where each token comes from some vocabulary V, e.g.,:

[I, love, cats, and, dogs]

• Natural language doesn't come as a sequence of tokens, but as just a string (concretely, sequence of Unicode characters):

I love cats and dogs

• A <u>tokenizer</u> converts any string into a sequence of tokens:

I love cats and dogs \Longrightarrow [I, love, cats, and, dogs]

Split by Space



- The simplest solution is to do: text.split(' ')
- This doesn't work for languages such as Chinese, where sentences are written without spaces between words:
 - 我今天去了商店: [I went to the store today.]
- Then there are languages like German that have long compound words:
 - Abwasserbehandlungsanlange: [Wastewater treatment plant]
- Even in English, there are hyphenated words (e.g., father-in-law) and contractions (e.g., don't), which should get split up.

What Makes a Good Tokenization?



- We don't want too many tokens:
 - The extreme case characters or bytes;
 - The sequence becomes difficult to model.
- We don't want too few tokens:
 - There won't be parameter sharing between words (e.g., should mother-in-law and father-in-law be completely different)?
 - This is especially problematic for morphologically rich languages (e.g., Arabic, Turkish, etc.).
- Each token should be a linguistically or statistically meaningful unit.



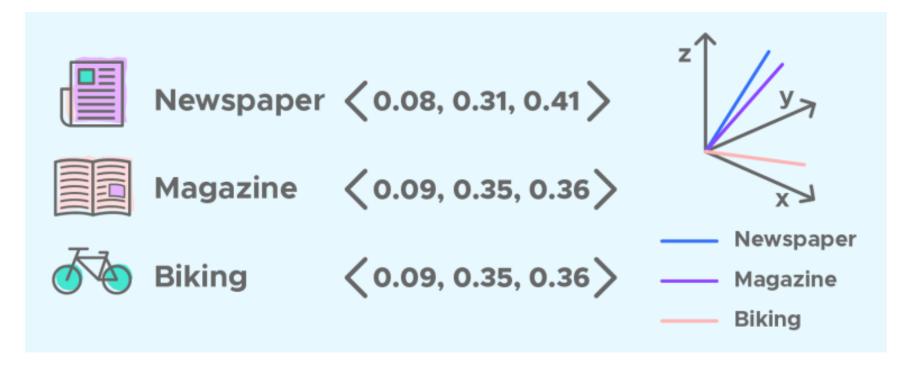


- Byte pair encoding (BPE)
 - Start with each character as its own token and combine tokens that cooccur a lot.
 - https://arxiv.org/pdf/1508.07909.pdf
- Unigram model (SentencePiece):
 - Rather than just splitting by frequency, a more "principled" approach is to define an objective function that captures what a good tokenization looks like.
 - https://arxiv.org/pdf/1804.10959.pdf





- Tokens can be represented as number index: $[I, love, cats, and, dogs] \Rightarrow [328, 793, 3989, 537, 3255, 269]$
- But indices are also meaningless.
- Represent words in a vector space
 - Vector distance ⇒ similarity.





LLM Categorization



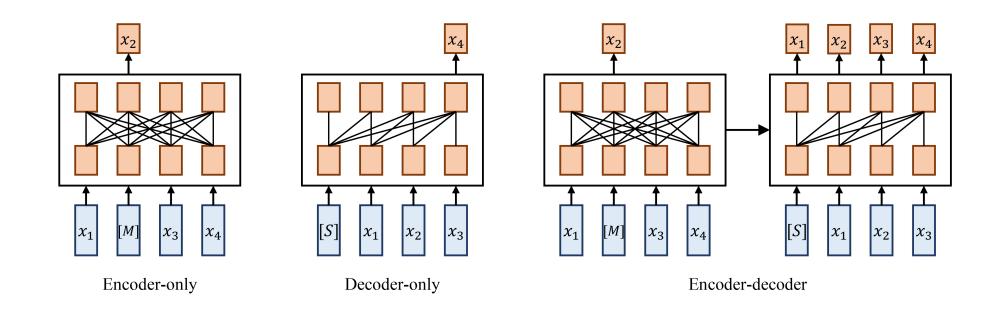


- Language model:
 - Associate a sequence of tokens with a corresponding sequence of contextual embeddings.
- Embedding function (analogous to a feature map for sequences):
 - $\emptyset: \mathcal{V}^L \to \mathbb{R}^{L \times D}$
 - A token sequence x_{1:L}[x₁, x₂, ..., x_L] ∈ V^L
 Map to Ø(x_{1:L}) ∈ ℝ^{L×D}
- For example, if D = 2:
 - [I, love, cats, and, dogs] \Longrightarrow [328, 793, 3989, 537, 3255, 269] \Longrightarrow

Types of language models



- Encoder-only models (BERT, RoBERTa, etc.)
- Encoder-decoder models (BART, T5, etc.)
- Decoder-only models (GPT-3, Llama-3, Deepseek-V3, etc.)







• Encoder-only models produce contextual embeddings but cannot be used directly to generate text:

$$x_{1:L} \Rightarrow \emptyset(x_{1:L})$$

- These contextual embeddings are generally used for classification tasks (sometimes boldly called natural language understanding tasks).
 - Example: sentiment classification: [[CLS],the,movie,was,great] ⇒ positive.
- Pros:
 - Contextual embedding for x_i can depend bidirectionally on both the left context $(x_{1:i-1})$ and the right context $(x_{i+1:L})$.
- Cons:
 - Cannot naturally generate completions.
 - Requires more ad-hoc training objectives (masked language modeling).

Decoder-only Models



- Decoder-only models are our standard autoregressive language models.
- Given a prompt $x_{1:i}$ produces both contextual embeddings and a distribution over next tokens x_{i+1} , and recursively, over the entire completion $x_{i+1:L}$:

$$x_{1:i} \Rightarrow \emptyset(x_{1:i}), p(x_{i+1}|x_{1:i})$$

- Example: text autocomplete
 - [[CLS],the,movie,was]⇒great
- Pro:
 - Can naturally generate completions.
 - Simple training objective (maximum likelihood).
- Con:
 - Contextual embedding for x_i can only depend **unidirectionally** on both the left context $(x_{1:i-1})$.

Encoder-decoder Models



• Encoder-decoder models can be the best of both worlds: they can use bidirectional contextual embeddings for the input $x_{1:L}$ and can generate the output $y_{1:L}$:

$$x_{1:L} \Rightarrow \emptyset(x_{1:L}), p(y_{1:L}|\emptyset(x_{1:L}))$$

- Example: table-to-text generation
 - [name,:,Clowns, |,eatType,:,coffee,shop]⇒[Clowns,is,a,coffee,shop].
- Pro:
 - Can naturally generate outputs.
- Con:
 - Requires more ad-hoc training objectives.



LLM Training Objectives

Decoder-only Model Training Objectives



- Recall that an autoregressive language model defines a conditional distribution: $p(x_i|x_{1:i-1})$
- Define it as follows:
 - Map $x_{1:i-1}$ to contextual embedding $\emptyset(x_{1:i-1}) \in \mathbb{R}^{(i-1) \times D}$;
 - Apply an embedding matrix $E \in \mathbb{R}^{D \times |\mathcal{V}|}$ to obtain scores for each token $\emptyset(x_{1:i-1})_{i-1}E \in \mathbb{R}^{|\mathcal{V}|}$ (where $\emptyset(x_{1:i-1})_{i-1} \in \mathbb{R}^D$);
 - Exponentiate and normalize it to produce the distribution over x_i .
- Put them together:

$$p(x_{i+1}|x_{1:i}) = \operatorname{softmax}(\emptyset(x_{1:i})_i E)$$





- Maximum likelihood. Let θ be all the parameters of large language models.
- Let \mathcal{D} be the training data consisting of a set of sequences. We can then follow the maximum likelihood principle and define the following negative log-likelihood objective function:

$$\mathcal{O}(\theta) = \sum_{x_{1:L \in \mathcal{D}}} -\log p_{\theta}(x_{1:L}) = \sum_{x_{1:L \in \mathcal{D}}} \sum_{i=1}^{L} -\log p_{\theta}(x_i|x_{1:i-1})$$

• Then we can use the SGD optimizers we have talked to optimize this loss function.



LLM Architecture Details

EmbedToken



- Convert sequences of tokens into sequences of vectors.
- EmbedToken does exactly this by looking up each token in an embedding matrix $E \in \mathbb{R}^{|\mathcal{V}| \times D}$, a parameter that will be learned from data.
- EmbedToken $(x_{1:L}: \mathcal{V}^L) \to \mathbb{R}^{L \times D}$:
 - Turns each token x_i in the sequence $x_{1:L}$ into a vector $E_{x_i} \in \mathbb{R}^D$;
 - Return $[E_{x_1}, E_{x_2}, \dots, E_{x_L}]$.
- These are *context-independent* word embeddings.
- Next the TransformerBlock(s) takes these context-independent embeddings and maps them into contextual embeddings.





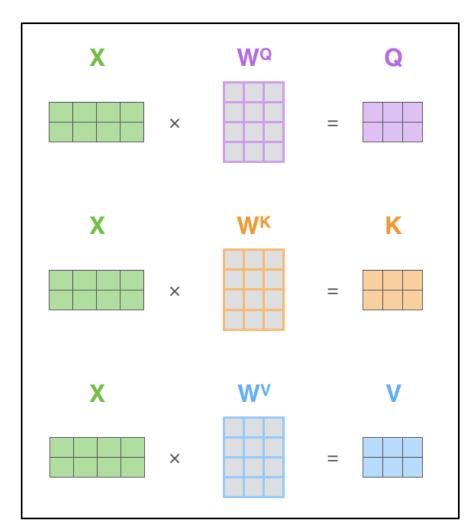
- TransformerBlock(s) takes these context-independent embeddings and maps them into contextual embeddings.
- TransformerBlocks $(X_{1:L}: R^{L \times D}) \to \mathbb{R}^{L \times D}$:
 - Process each element $X_i \in \mathbb{R}^D$ in the sequence $X_{1:L} \in \mathbb{R}^{L \times D}$ with respect to other elements.
- TransformerBlock(s) are the building blocks of decoder-only (GPT-2, GPT-3), encoder-only (BERT, RoBERTa), and decoder-encoder (BART, T5) models.



Attention Mechanism-1



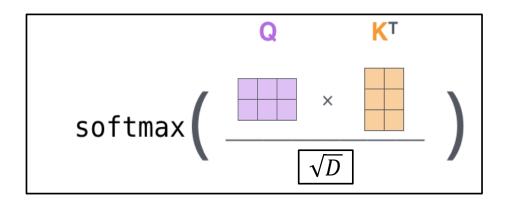
- **First step**: in each transformer block, for each token, we create a query vector, a key vector, and a value vector by multiplying the embedding by three weight matrices.
- Formally, for each token $X_i \in \mathbb{R}^D$:
 - Query: $Q_i = X_i \times W^Q$
 - key: $K_i = X_i \times W^K$
 - Value: $V_i = X_i \times W^V$
- In the tensor representation for sequence $X_{1:L} \in \mathbb{R}^{L \times D}$:
 - Query: $Q = Q_{1:L} = X_{1:L} \times W^Q$
 - key: $K = K_{1:L} = X_{1:L} \times W^K$
 - Value: $V = V_{1:L} = X_{1:L} \times W^V$







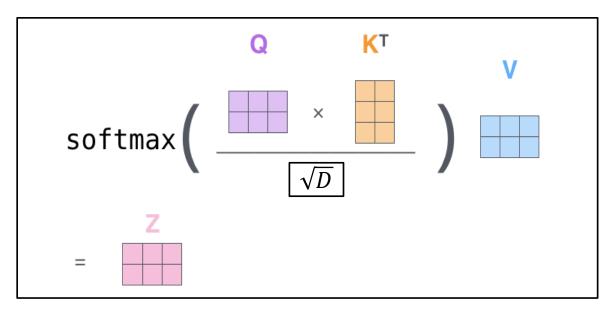
- <u>Second step</u>: Calculate a score determining how much focus to place on other parts of the input sentence as we encode a token at a certain position.
- Calculated by:
 - Taking the dot product of the query vector with the key vector of the respective word we're scoring;
 - Divide the scores by the square root of the dimension of the key vectors;
 - Conduct a softmax operation.
- score = softmax($\frac{QK^T}{\sqrt{D}}$)



Attention Mechanism-3



- Third step: combine the value and the score.
 - $Z = att = softmax \left(\frac{QK^T}{\sqrt{D}}\right)V$
- Multi-head Attention: there can be multiple aspects (e.g., syntax, semantics) we would want to match on.
- To accommodate this, we can simultaneously have multiple attention heads (e.g. n_H heads) and simply combine their outputs, e.g.
 - $Z = [att^1, att^2, ..., att^{n_H}]$
- The attention output will be:
 - Out = ZW^O



Feedforward Layer



- After the attention layer, the output is put to a feed-forward neural network, then sends out the output upwards to the next encoder.
 - $X'_{1:L} = \text{relu}(\text{Out}W^1)W^2$
 - W^1 , W^2 are two weight matrices;
 - $X'_{1:L}$ is the output embedding for the current layer and the input of the next layer.
- Summarize a common weight dimension in one **TransformerBlock**:
 - Attention layer: W^Q , W^K , W^V , $W^O \in \mathbb{R}^{D \times D}$
 - Feedforward layer: $W^1 \in \mathbb{R}^{D \times 4D}$, $W^2 \in \mathbb{R}^{4D \times D}$

TransformerBlocks $(X \in R^{L \times D}) \rightarrow X' \in \mathbb{R}^{L \times D}$



- *L* is the sequence length;
- *D* is the model dimension;
- Multi-head attention: $D = n_H \times H$
- *H* is the head dimension;
- n_h is the number of heads.

Computation	Input	Output
$Q = XW^Q$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^Q \in \mathbb{R}^{D \times D}$	$Q \in \mathbb{R}^{L \times D}$
$K = XW^K$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^K \in \mathbb{R}^{D \times D}$	$K \in \mathbb{R}^{L \times D}$
$V = XW^V$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^V \in \mathbb{R}^{D \times D}$	$V \in \mathbb{R}^{L \times D}$
$[Q^1, Q^2 \dots, Q^{n_H}] = Partion_{-1}(Q)$	$Q \in \mathbb{R}^{L \times D}$	$Q^h \in \mathbb{R}^{L \times H}, h = 1, \dots n_H$
$[K^1, K^2 \dots, K^{n_H}] = Partion_{-1}(K)$	$K \in \mathbb{R}^{L \times D}$	$K^h \in \mathbb{R}^{L \times H}, h = 1, \dots n_H$
$[V^1, V^2 \dots, V^{n_H}] = Partion_{-1}(V)$	$V \in \mathbb{R}^{L \times D}$	$V^h \in \mathbb{R}^{L \times H}, h = 1, \dots n_H$
$score^h = softmax(\frac{Q^h K^{h^T}}{\sqrt{D}}), i = 1, n_H$	$Q^h, K^h \in \mathbb{R}^{L \times H}$	$score^h \in \mathbb{R}^{L \times L}$
$Z^h = \operatorname{score}^h V^h$, $h = 1, n_H$	$score^h \in \mathbb{R}^{L \times L}, V^h \in \mathbb{R}^{L \times H}$	$Z^h \in \mathbb{R}^{L \times H}$
$Z = \text{Merge}_{-1} ([Z^1, Z^2, Z^{n_H}])$	$Z^h \in \mathbb{R}^{L \times H}$, $h = 1, \dots n_H$	$Z \in \mathbb{R}^{L \times D}$
$Out = ZW^O$	$Z \in \mathbb{R}^{L imes D}$, $\mathbb{W}^O \in \mathbb{R}^{D imes D}$	Out $\in \mathbb{R}^{L \times D}$
$A = \text{Out } W^1$	Out $\in \mathbb{R}^{L \times D}$, $\mathbb{W}^1 \in \mathbb{R}^{D \times 4D}$	$A \in \mathbb{R}^{L \times 4D}$
$A' = \operatorname{relu}(A)$	$A \in \mathbb{R}^{L \times 4D}$	$A' \in \mathbb{R}^{L \times 4D}$
$X' = A'W^2$	$A' \in \mathbb{R}^{L \times 4D}$, $\mathbb{W}^2 \in \mathbb{R}^{4D \times D}$	$X' \in \mathbb{R}^{L \times D}$

Other Components



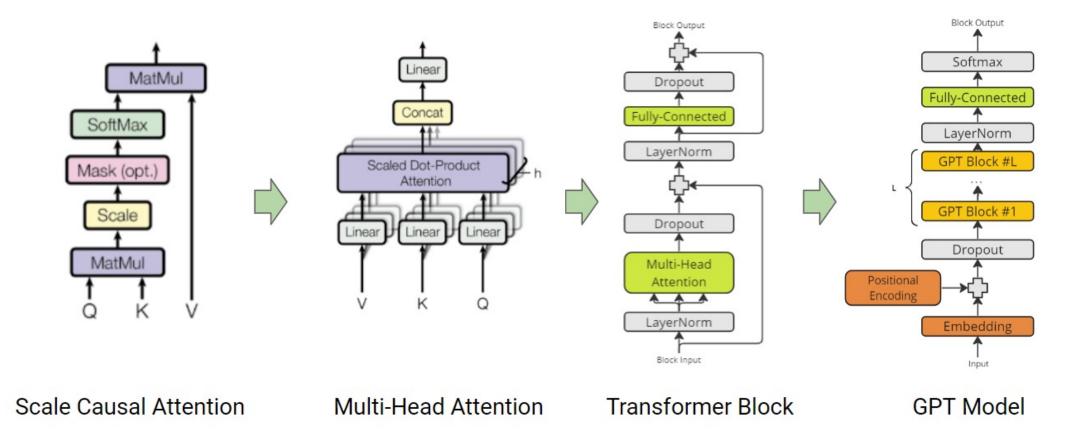
- Residual connections:
 - Instead of simply return TransformerBlock($X_{1:L}$)
 - Return: $X_{1:L}$ + TransformerBlock($X_{1:L}$)
- Layer normalization:
 - LayerNorm $(X_{1:L}) = \alpha \frac{X_{1:L} \mu}{\sigma} + \beta$
 - μ is the mean; σ is the standard deviation.
 - α and β are learnable parameters.
- Positional embeddings:
 - So far, the embedding of a token doesn't depend on where it occurs in the sequence, which is not sensible. (PosEmb $\in \mathbb{R}^{L \times D}$)

PosEmb
$$(i, 2j) = \sin(\frac{i}{10000^{2j/D}})$$
PosEmb $(i, 2j + 1) = \cos(\frac{i}{10000^{2j/D}})$

- Where $i = 1, ..., L, j = 1, ..., \frac{D}{2}$
- $X_{1:L} = X_{1:L} + \text{PosEmb before computing } Q_{1:L}, K_{1:L}, V_{1:L}$.

Put Them Together





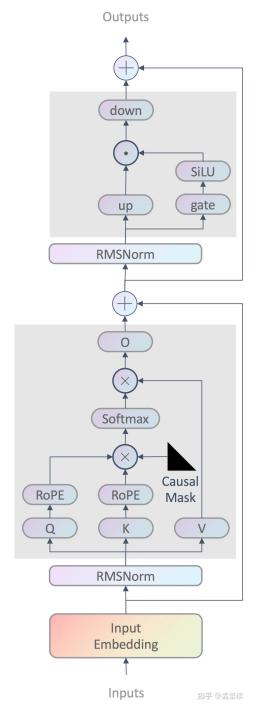


LLM Architecture Case Study



Llama-3 Block Overview

- RMSNorm (Root Mean Square Norm);
- RoPE (Rotary Position Embedding);
- GQA (Group Query Attention);
- SiLU activation function in MLP.





Llama-3 RMSNorm

- RMSNorm: RMSNorm $(X_{1:L}) = \alpha \frac{X_{1:L}}{\sqrt{\mu^2 + \epsilon}}$
 - μ is the mean.
 - 40% Speed-up compared with LayerNorm.

RMSNorm

CLASS torch.nn.RMSNorm(normalized_shape, eps=None, elementwise_affine=True, device=None, dtype=None) [SOURCE]

Applies Root Mean Square Layer Normalization over a mini-batch of inputs.

This layer implements the operation as described in the paper Root Mean Square Layer Normalization

$$y_i = rac{x_i}{ ext{RMS}(x)} * \gamma_i, \quad ext{where} \quad ext{RMS}(x) = \sqrt{\epsilon + rac{1}{n} \sum_{i=1}^n x_i^2}$$

The RMS is taken over the last D dimensions, where D is the dimension of normalized_shape. For example, if normalized_shape is (3, 5) (a 2-dimensional shape), the RMS is computed over the last 2 dimensions of the input.

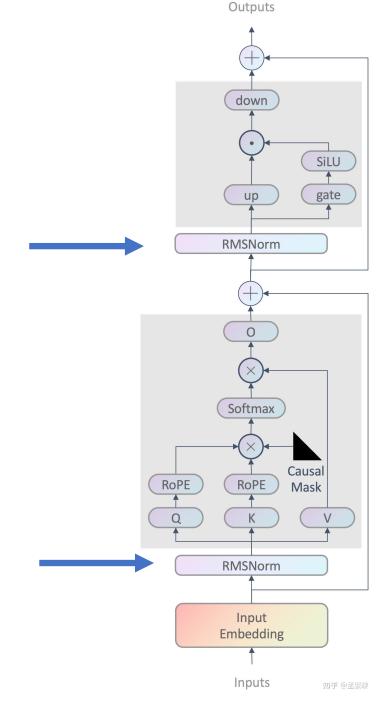
Parameters

 normalized_shape (int or list or torch.Size) – input shape from an expected input of size

 $[* \times normalized_shape[0] \times normalized_shape[1] \times \ldots \times normalized_shape[-1]$

If a single integer is used, it is treated as a singleton list, and this module will normalize over the last dimension which is expected to be of that specific size.

- eps (Optional[float]) a value added to the denominator for numerical stability. Default: torch.finfo(x.dtype).eps()
- elementwise_affine (bool) a boolean value that when set to True, this module has learnable perelement affine parameters initialized to ones (for weights). Default: True.





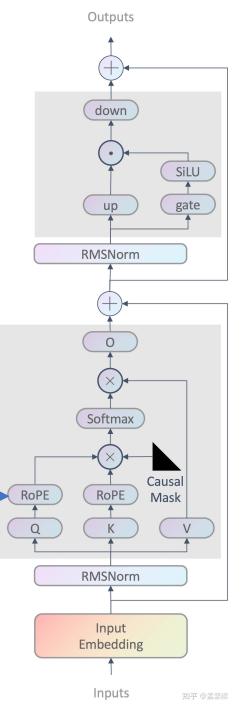
Llama-3 RoPE



- RoPE incorporates both absolute and relative positional information.
- Computation efficient implementation transform a position *i*:

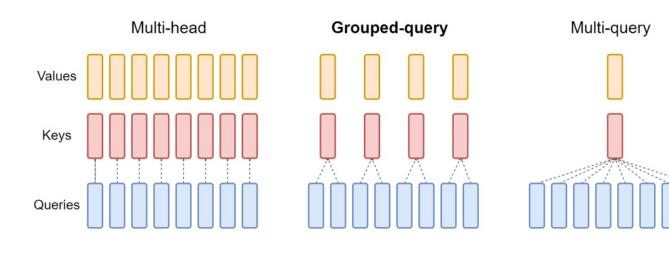
$$\begin{pmatrix} X_{i,1} \\ X_{i,2} \\ X_{i,1} \\ X_{i,1} \\ \vdots \\ X_{i,D-1} \\ X_{i,D} \end{pmatrix} \otimes \begin{pmatrix} \cos i\theta_1 \\ \cos i\theta_2 \\ \cos i\theta_2 \\ \vdots \\ \cos i\theta_{D/2} \\ \cos i\theta_{D/2} \end{pmatrix} + \begin{pmatrix} -X_{i,2} \\ X_{i,1} \\ -X_{i,4} \\ X_{i,3} \\ \vdots \\ -X_{i,D} \\ X_{i,D-1} \end{pmatrix} \otimes \begin{pmatrix} \sin i\theta_1 \\ \sin i\theta_2 \\ \sin i\theta_2 \\ \sin i\theta_2 \\ \vdots \\ \sin i\theta_{D/2} \\ \sin i\theta_{D/2} \end{pmatrix}$$

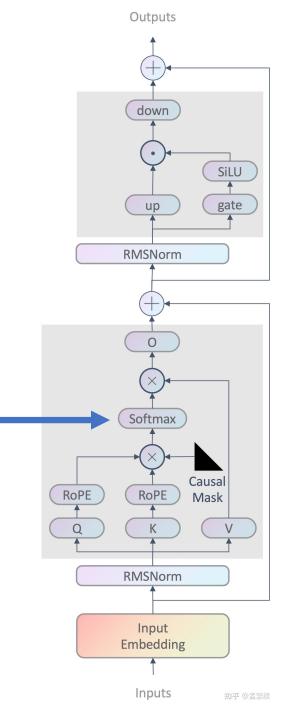
- 🛇 indicates element-wise multiplication;
- $\theta_i = 10000^{-\frac{2j}{D}}$
- https://arxiv.org/pdf/2104.09864



Llama-3 GQA

• Replace multi-head attention with grouped-query attention.





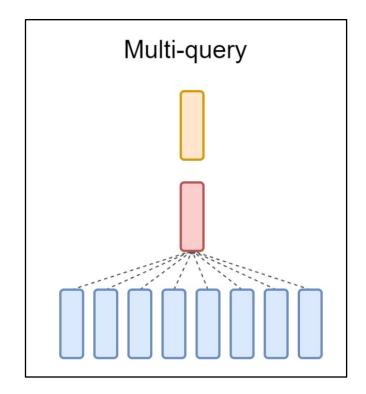






- The idea is simple yet effective:
 - Use multiple query heads but only a single key and value head.

Computation	Input	Output
$Q = XW^Q$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^Q \in \mathbb{R}^{D \times D}$	$Q \in \mathbb{R}^{L \times D}$
$K = XW^K$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^K \in \mathbb{R}^{D \times H}$	$K \in \mathbb{R}^{L \times H}$
$V = XW^V$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^V \in \mathbb{R}^{D \times H}$	$V \in \mathbb{R}^{L \times H}$
$[Q^1,Q^2\ldots,Q^{n_H}]=\mathrm{Partition}_{-1}(Q)$	$Q \in \mathbb{R}^{L \times D}$	$Q^h \in \mathbb{R}^{L \times H}$, $h = 1, \dots n_H$
$score^{h} = softmax(\frac{Q^{h}K^{T}}{\sqrt{D}}), h = 1, n_{H}$	$Q^h, K \in \mathbb{R}^{L \times H}$	$score^h \in \mathbb{R}^{L \times L}$
$Z^h = \operatorname{score}^h V, h = 1, n_H$	$score^h \in \mathbb{R}^{L \times L}, V \in \mathbb{R}^{L \times H}$	$Z^h \in \mathbb{R}^{L \times H}$

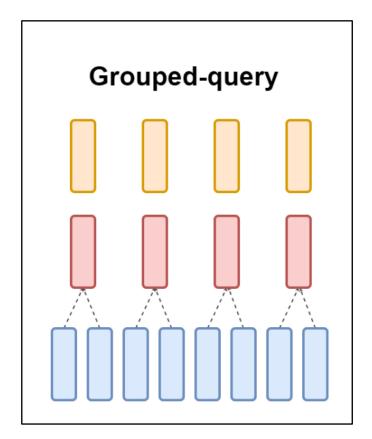






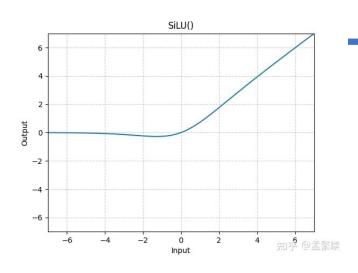
- The trade-off between MHA and MQA:
 - Divide query heads into *g* groups, each sharing a single key head and value head;
 - MHA: $g = n_H$; MQG: g = 1.

Computation	Input	Output
$Q = XW^Q$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^Q \in \mathbb{R}^{D \times D}$	$Q \in \mathbb{R}^{L \times D}$
$K = XW^K$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^K \in \mathbb{R}^{D \times gH}$	$K \in \mathbb{R}^{L \times gH}$
$V = XW^V$	$X \in \mathbb{R}^{L \times D}$, $\mathbb{W}^V \in \mathbb{R}^{D \times gH}$	$V \in \mathbb{R}^{L \times gH}$
$[Q^1,Q^2\ldots,Q^{n_H}]=\mathrm{Partition}_{-1}(Q)$	$Q \in \mathbb{R}^{L \times D}$	$Q^h \in \mathbb{R}^{L \times H}, h = 1, \dots n_{\mathrm{H}}$
$[K^1, K^2 \dots, K^g] = Partition_{-1}(K)$	$K \in \mathbb{R}^{L \times gH}$	$K^h \in \mathbb{R}^{L \times H}, h = 1, \dots g$
$[V^1, V^2 \dots, V^g] = Partition_{-1}(V)$	$V \in \mathbb{R}^{L \times gH}$	$V^h \in \mathbb{R}^{L \times H}, h = 1, \dots g$
$score^{h} = softmax(\frac{Q^{h}K^{[h/g]^{T}}}{\sqrt{D}}), h = 1, n_{H}$	$Q^h, K^{\lfloor h/g \rfloor} \in \mathbb{R}^{L \times H}$	$score^h \in \mathbb{R}^{L \times L}$
$Z^h = \operatorname{score}^h V^{\lfloor h/g \rfloor}, h = 1, \dots n_H$	$score^h \in \mathbb{R}^{L \times L}, V^{\lfloor h/g \rfloor} \in \mathbb{R}^{L \times H}$	$Z^h \in \mathbb{R}^{L \times H}$

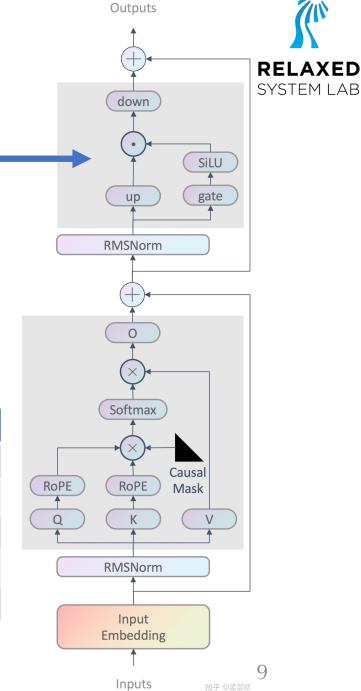


Llama-3 SiLU MLP

• Empirically shown to enhance model quality in various tasks.



Computation	Input	Output
$A = \text{Out } W^1$	Out $\in \mathbb{R}^{L \times D}$, $\mathbb{W}^1 \in \mathbb{R}^{D \times 4D}$	$A \in \mathbb{R}^{L \times 4D}$
$B = \text{Out}W^2$	Out $\in \mathbb{R}^{L \times D}$, $\mathbb{W}^2 \in \mathbb{R}^{D \times 4D}$	$B \in \mathbb{R}^{L \times 4D}$
B' = SiLU(B)	$B \in \mathbb{R}^{L \times 4D}$	$B' \in \mathbb{R}^{L \times 4D}$
$B^{\prime\prime}=A{\otimes}B^{\prime}$	$A \in \mathbb{R}^{L \times 4D}$, $B' \in \mathbb{R}^{L \times 4D}$	$B^{\prime\prime} \in \mathbb{R}^{L \times 4D}$
$X' = B''W^2$	$B^{\prime\prime} \in \mathbb{R}^{L \times 4D}$, $\mathbb{W}^3 \in \mathbb{R}^{4D \times D}$	$X' \in \mathbb{R}^{L \times D}$



References



- https://scholar.harvard.edu/sites/scholar.harvard.edu/files/binxuw/files/mlfs_tutorial_nlp_transformer_ssl_updated.pdf
- https://jalammar.github.io/illustrated-transformer/
- https://stanford-cs324.github.io/winter2022/lectures/introduction/
- https://stanford-cs324.github.io/winter2022/lectures/modeling/
- https://stanford-cs324.github.io/winter2022/lectures/training/
- https://zhuanlan.zhihu.com/p/636784644
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