Quick Announcements

- Gradescope is now live for HW1. Find the link for it from Canvas.
- Upload a requirements.txt file to Gradescope if your code needs non-standard packages.
- Office hours on the course website have been updated

Architecture Advancement on Transformers

Large Language Models: Methods and Applications

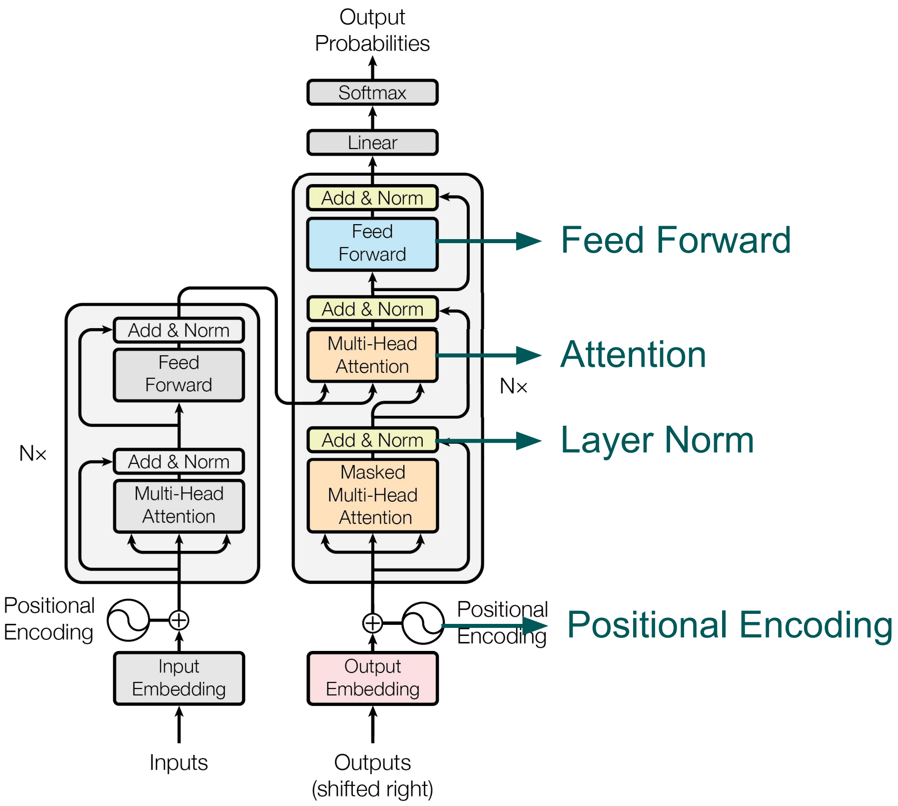
Daphne Ippolito and Chenyan Xiong

Learning Objectives

An overview of recent architecture advancements on top of Transformers

- A clear grasp on the details of new architectures
- Understand the motivation and benefits of each architecture upgrades
- Apply the right architecture specifications for target scenarios
- [Optional] Explore new architecture designs in your research

Places for Improvements



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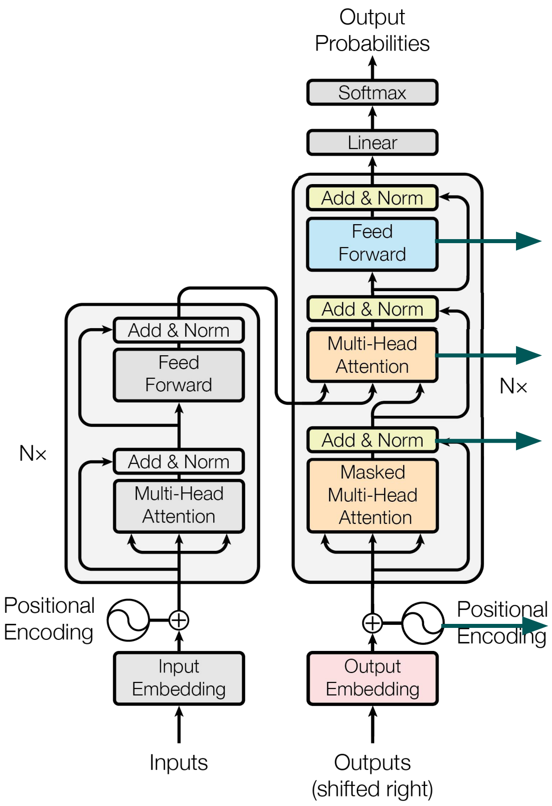

Feed Forward: Activations and Bilinear Layers

Attention

Layer Norm

Positional Encoding

Feed Forward: Activations and Bilinear Layers

Variants of linear FFN Layers (omitting bias):

$$\text{FFN}_{\text{RELU}}(x) = \text{RELU}(\,x\mathbf{W}_1)\mathbf{W}_2;\ \text{RELU}(\,x\mathbf{W}_1) = \max(0, x\mathbf{W}_1)\mathbf{W}_2$$

[1] Hendrycks and Gimpel. 2016. Gaussian Error Linear Units.
[2] Ramachandran et al. 2017. Searching for Activation Functions.

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$$\mathrm{FFN}_{\mathrm{GELU}}(x) = \mathrm{GELU}(x\mathbf{W}_1)\mathbf{W}_2; \mathrm{GELU}(x\mathbf{W}_1) = xP(X < x) = x\Phi(x)$$

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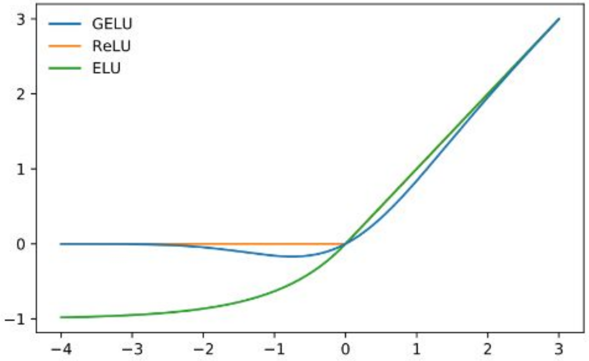

GELU Activation [1]

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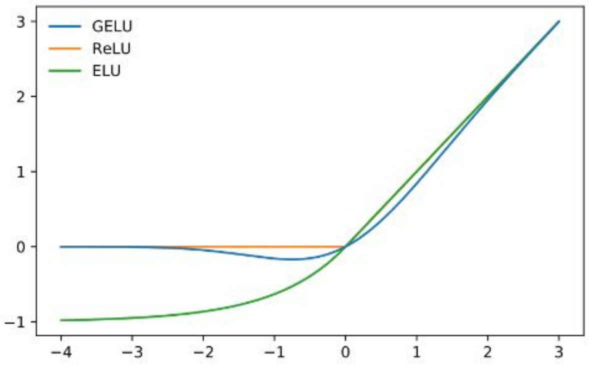
$$\mathrm{FFN}_{\mathrm{Switch}}(x) = \mathrm{Swish}_1(\,x\mathbf{W}_1)\mathbf{W}_2; \mathrm{Swish}_\beta(\,x\mathbf{W}_1) = x\mathrm{Sigmod}(\beta x)$$



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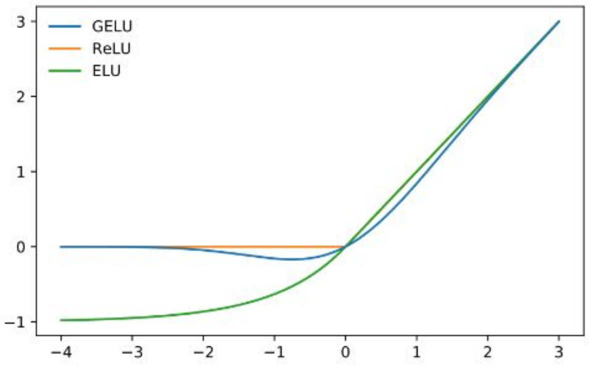

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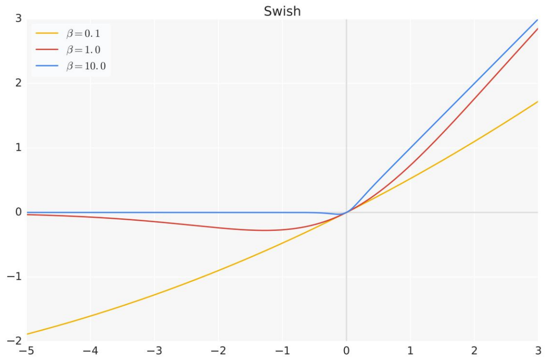

Switch Activation [2]

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Feed Forward: Activations and Bilinear Layers

Bilinear FFNs (Omitting Bias):

$\mathrm{FFN}_{\mathrm{Bilinear}}(x) = (x\mathbf{W} \cdot x\mathbf{V})\mathbf{W}_2$. Two FFN with componentwise product

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With reduced hidden dimension of the projections to keep parameter count the same

Training Steps	65,536	524,288
$\mathrm{FFN}_{\mathrm{ReLU}}(baseline)$	1.997 (0.005)	1.677
$\mathrm{FFN}_{\mathrm{GELU}}$	1.983 (0.005)	1.679
$\mathrm{FFN}_{\mathrm{Swish}}$	1.994 (0.003)	1.683
$\mathrm{FFN}_{\mathrm{GLU}}$	1.982 (0.006)	1.663
$\mathrm{FFN}_{\mathrm{Bilinear}}$	1.960 (0.005)	1.648
$\mathrm{FFN}_{\mathrm{GEGLU}}$	**1.942** (0.004)	**1.633**
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Improved speed-quality

T5 base Perplexity at Pretraining Steps [3]

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"We offer no explanation as to why these architectures seem to work; we attribute their success, as all else, to divine benevolence"---Noam Shazeer. 2017

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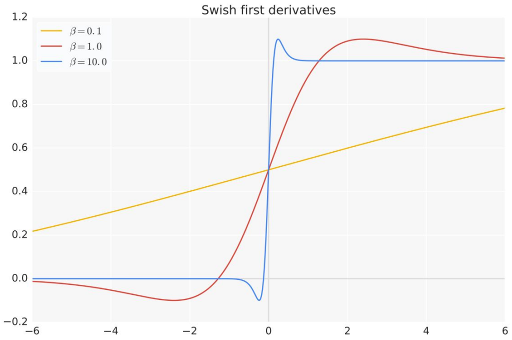
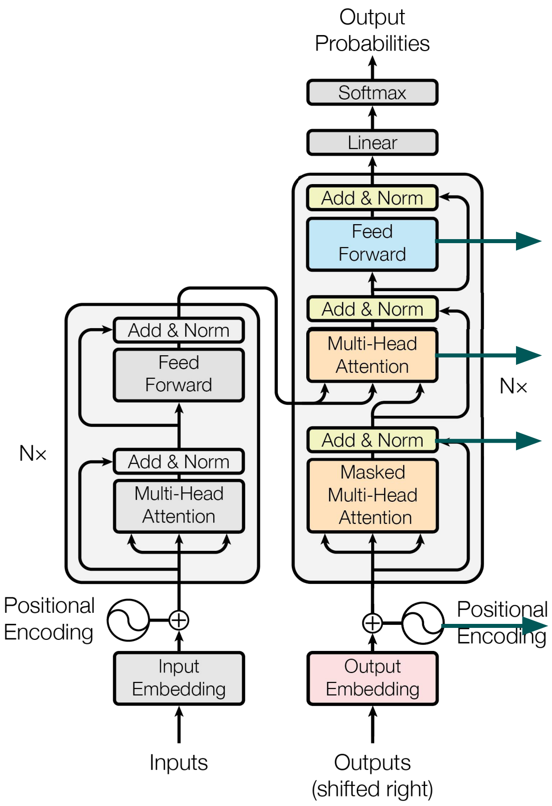


Switch Gradients [2]

Places for Improvements



Feed Forward: Activations and Bilinear Layers

Attention: Efficient Attention Mechanisms

Layer Norm

Positional Encoding

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Standard Multi-Head Attention

$$\mathrm{head}_1 = \mathrm{Attention}\left(\mathbf{Q}\mathbf{W}_1^Q, \mathbf{K}\mathbf{W}_1^K, \mathbf{V}\mathbf{W}_1^V\right)$$
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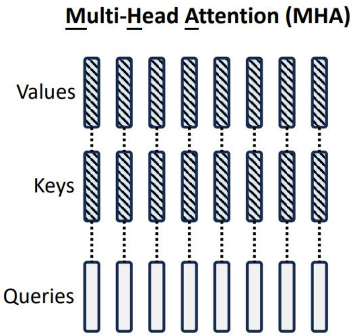

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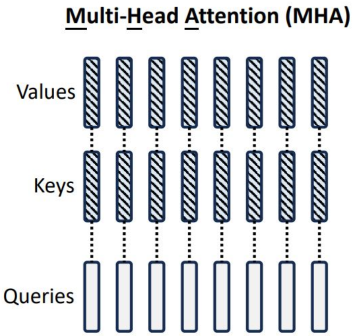

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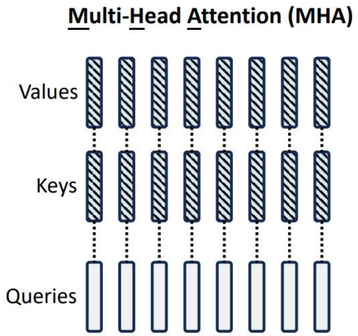
Huge memory consumption during inference. Needs to keep one K, V for each layer and each position



Attention: Efficient Attention Mechanisms

Grouped-Query Attention: Divide Q in G groups, and share K, V in the same group [4]

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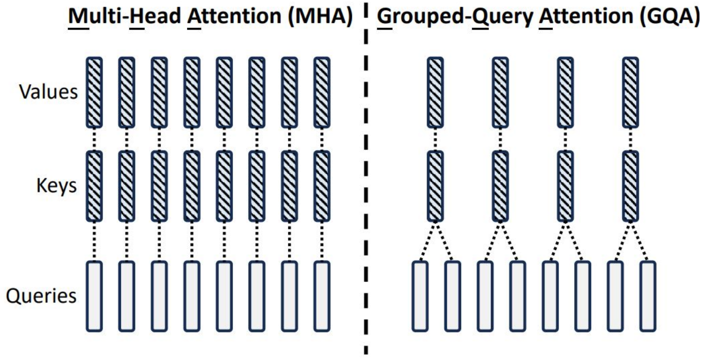

[4] Ainslie et al. 2023. GQA: Training Generalized Multi-Query Transformer Models from Multi-Head Checkpoints

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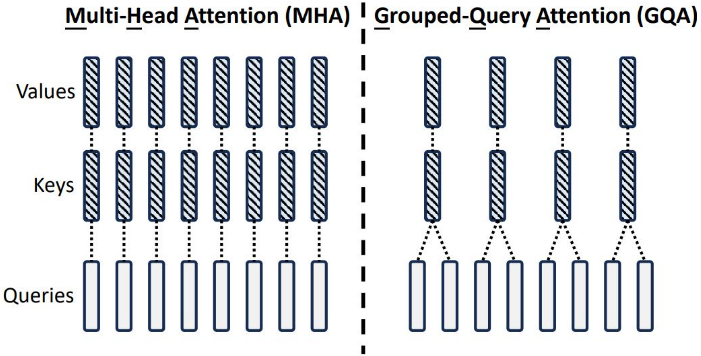

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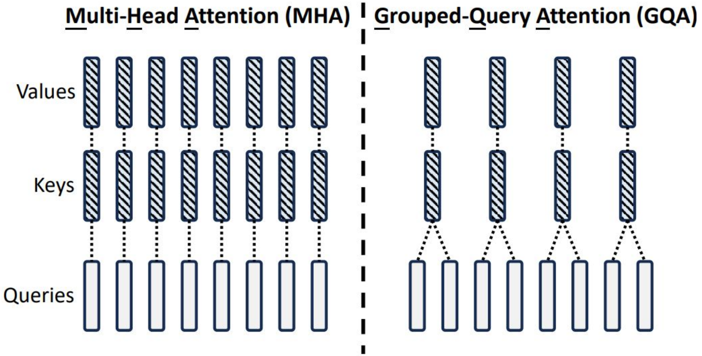
Reduce K, V cache storage to group sizes



Attention: Efficient Attention Mechanisms

Multi-Query Attention: Single K, V for all Q heads [5]

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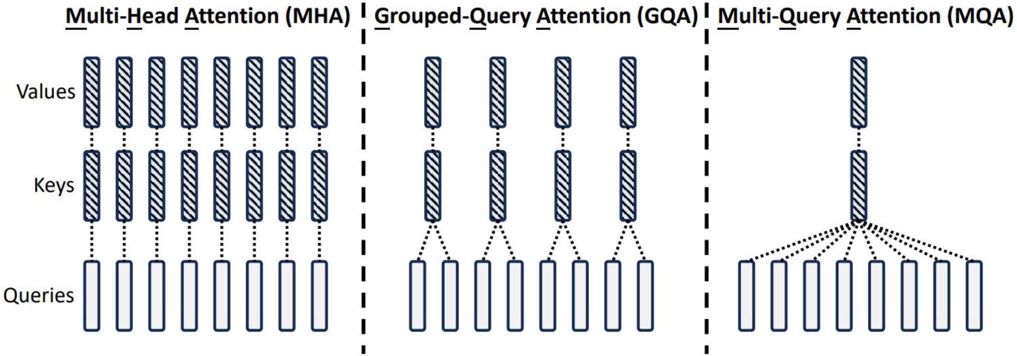

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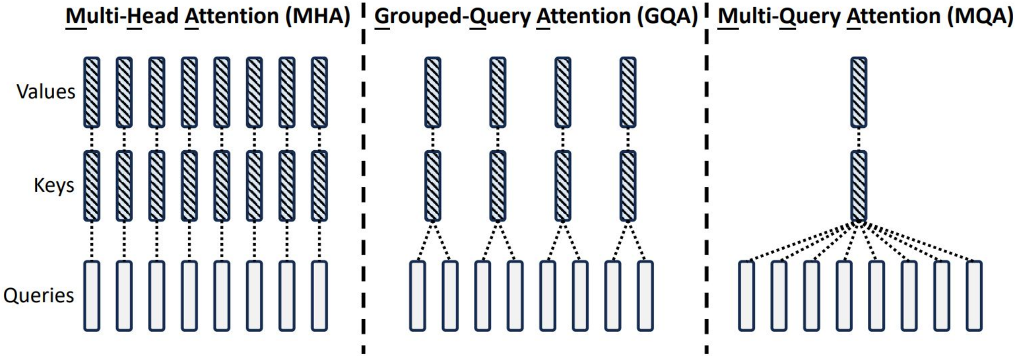

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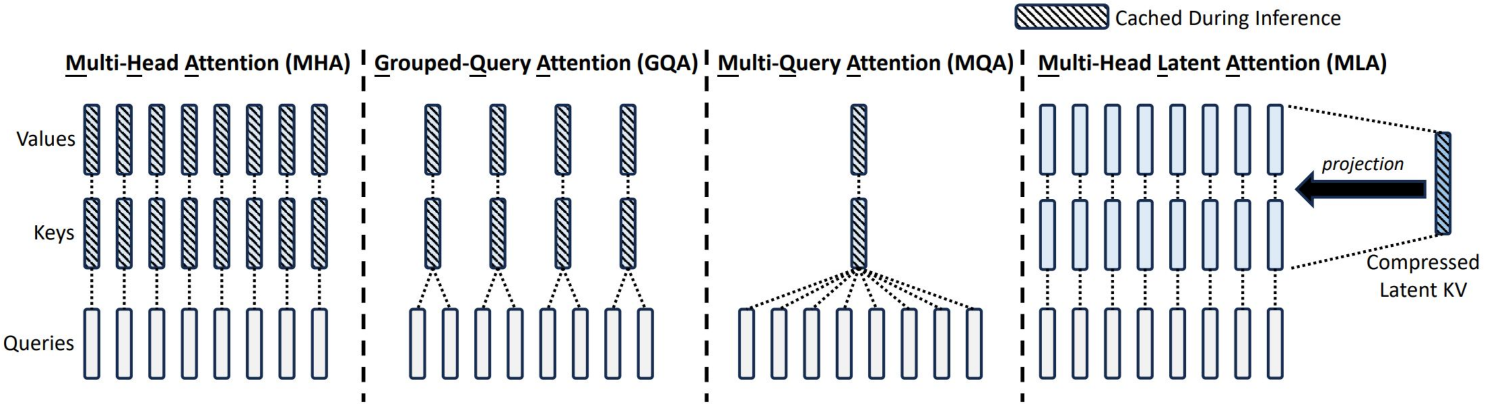
Attention: Efficient Attention Mechanisms

Multi-Head Latent Attention: Project K, V into a lower dimension latent vector [6]

$$\boldsymbol{k}_t = \mathbf{W}^{UK} \mathbf{c}_t^{KV}$$
$$\boldsymbol{v}_t = \mathbf{W}^{UV} \mathbf{c}_t^{KV}$$

Recovery of k, v can be merged with q in attention layer operations

$$\mathbf{c}_t^{KV} = \mathbf{W}^{DKV} \mathbf{h}_t$$ Only latent vector to store



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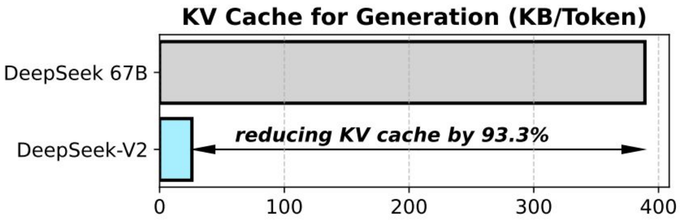

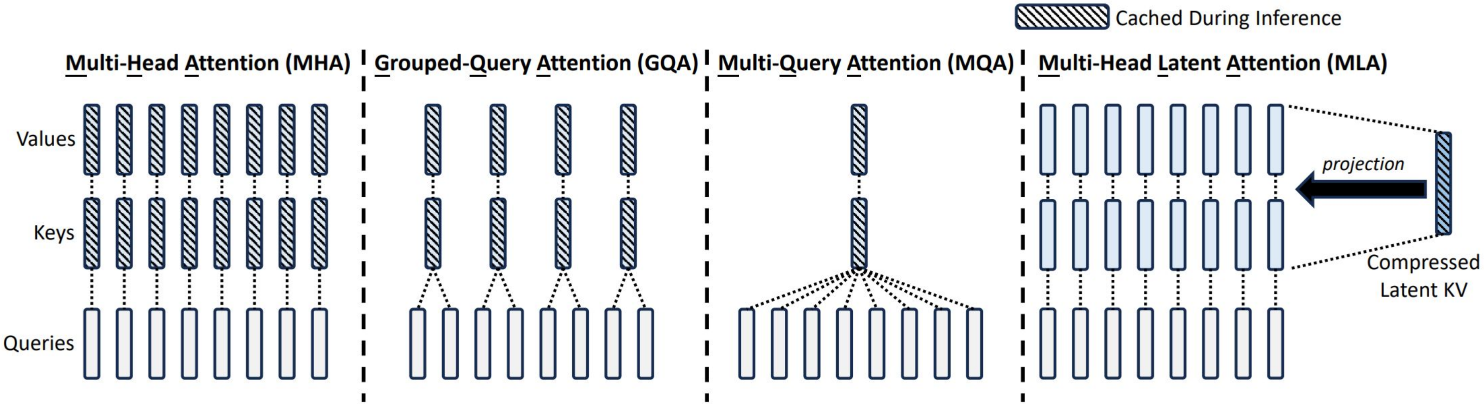

Attention: Efficient Attention Mechanisms

How to use efficient attention mechanisms:

- Pretraining directly with updated architecture
- Or use it as a compression method to speed up a rich multi-head attention model

[4] Ainslie et al. 2023. GQA: Training Generalized Multi-Query Transformer Models from Multi-Head Checkpoints

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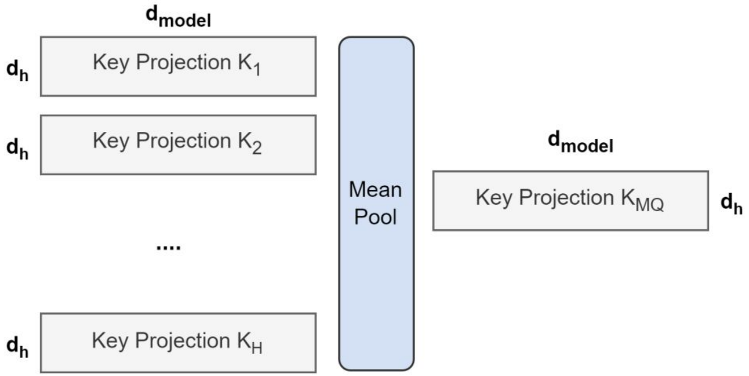

Mean Pooling Multi-Head Attention to Grouped-Query Attention [4]

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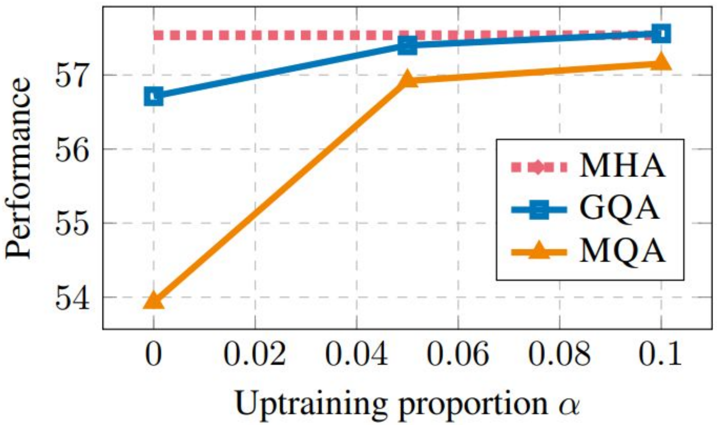
Attention: Efficient Attention Mechanisms

Performance:

- Recovering similar effectiveness as multi-head attention
- Significantly improve generation speed



Performance of Grouped-Query Attention Adapted from Multi-Head Attention [4]

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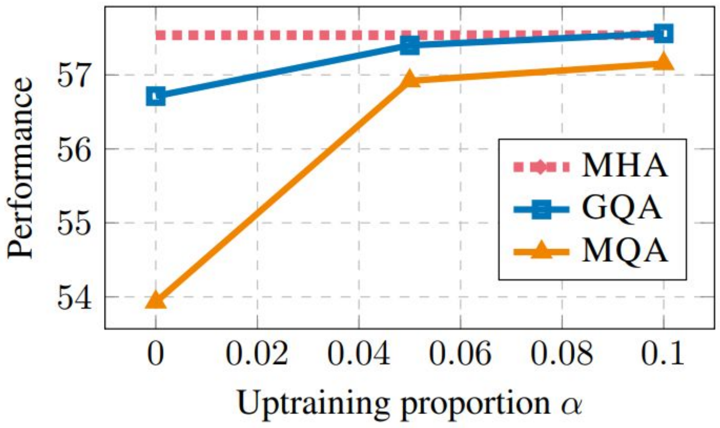
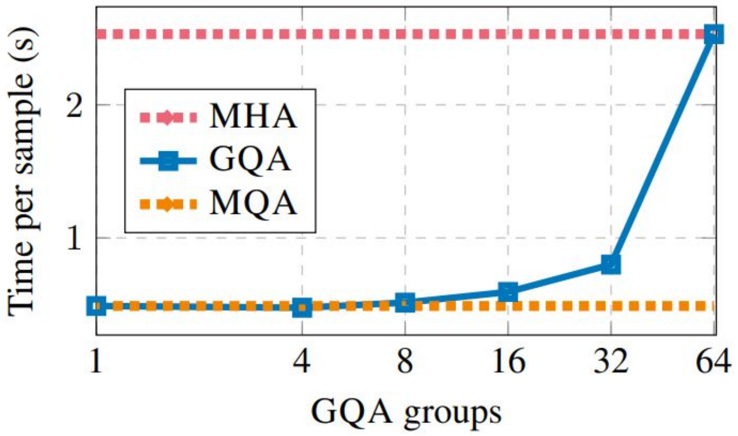
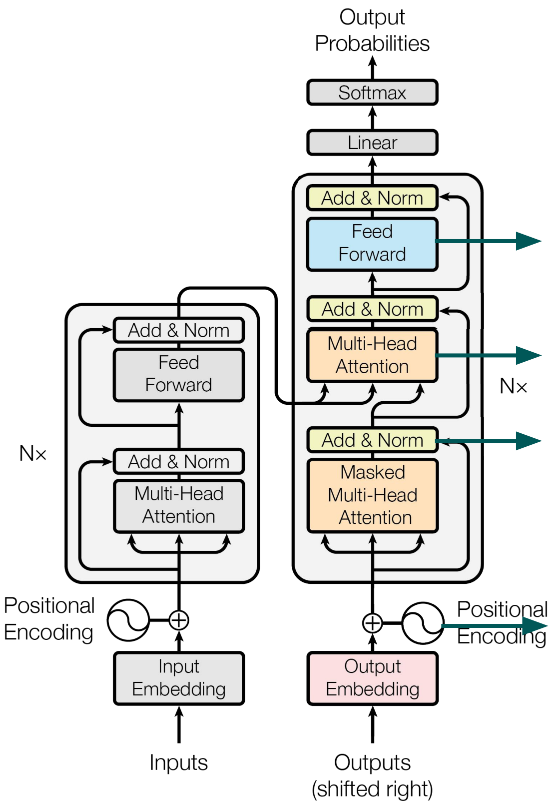


Performance of Grouped-Query Attention Adapted from Multi-Head Attention [4]



Generation Efficiency with Grouped-Query Attention [4]

Places for Improvements



Feed Forward: New Activations and Bilinear Layers

Attention: Efficient Attention Mechanisms

Layer Norm: Simpler and Stabler Layer Norms

Positional Encoding

Layernorm: Simpler and Stabler Layernorms

The Layer Normalization Layer [5]:

$$\mathrm{LN}(x_i) = \frac{(x_i - \mu)}{\sigma} g_i; \quad \mu = \frac{1}{d}\sum_i x_i, \sigma = \sqrt{\frac{1}{d}\sum_i (x_i - \mu)^2}$$

Learnable parameter started from 1

Align the outputs to standard distributions to improve training convergence and stability

[5] Ba et al. 2016. Layer Normalization
[6] Xiong et al. 2020. On Layer Normalization in the Transformer Architecture

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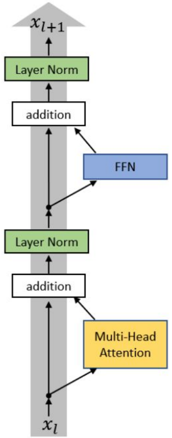

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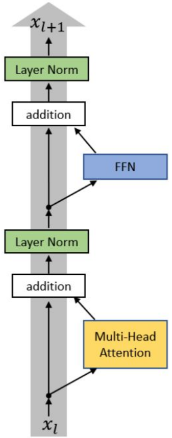

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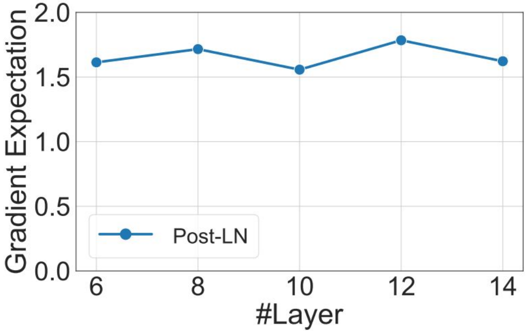

Large gradient L2 norm, leading to unstable training at large scale [6]

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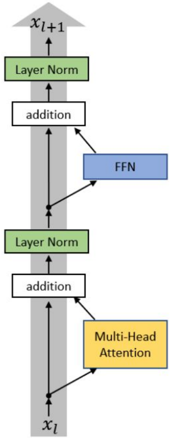

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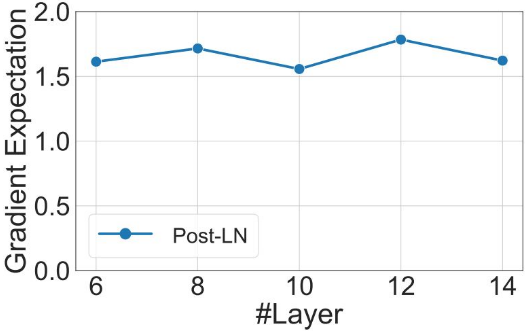

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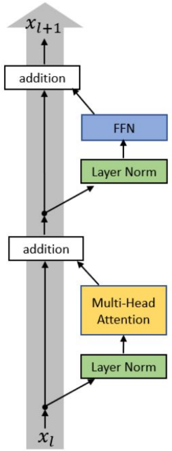

Pre-LN: Before Residual Sum

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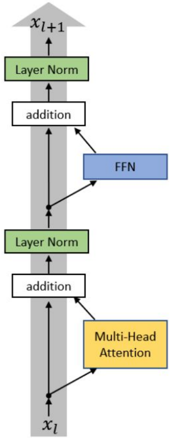

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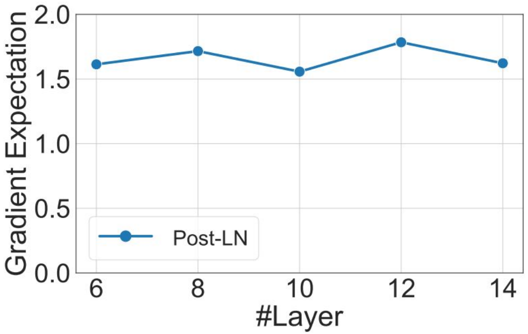

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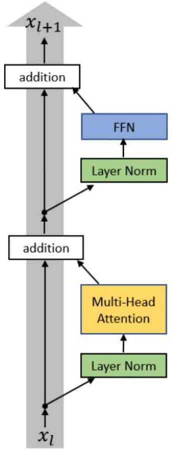

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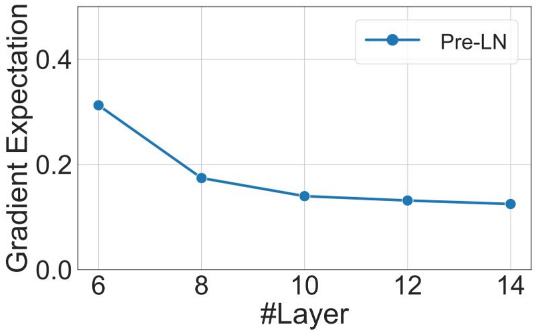

Lower gradient L2 norm, improved training stability [6]

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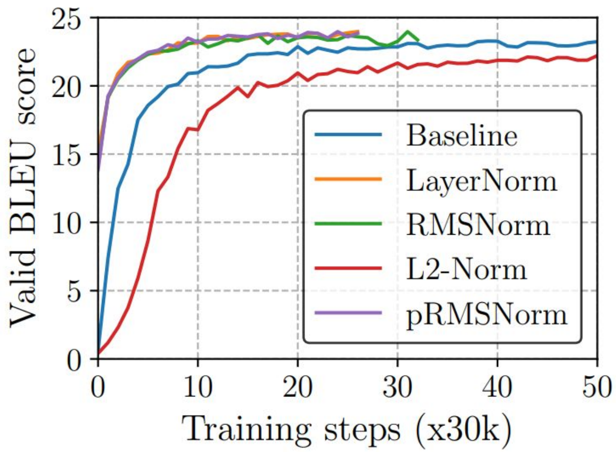

Better Convergence Rate on Machine Translation and Many NLP Tasks [7]

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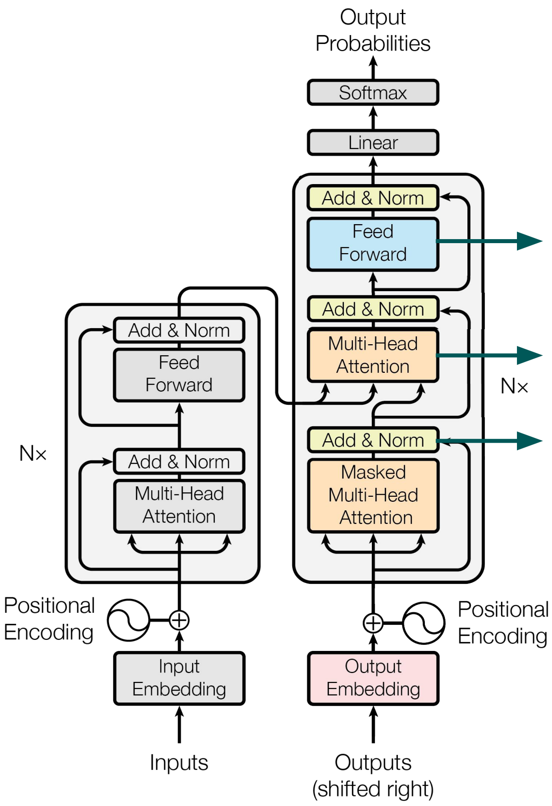
Places for Improvements: Recap



Feed Forward: New Activations and Bilinear Layers

Improving Speed-Quality with Different Shapes

Attention: Efficient Attention Mechanisms

Trade Off Some Quality for (Inference) Speed

Layer Norm: Simpler and Stabler Layer Norms

Improving Training Speed and Robustness with Simplicity

These architecture upgrades are adapted in most recent public production LLMs

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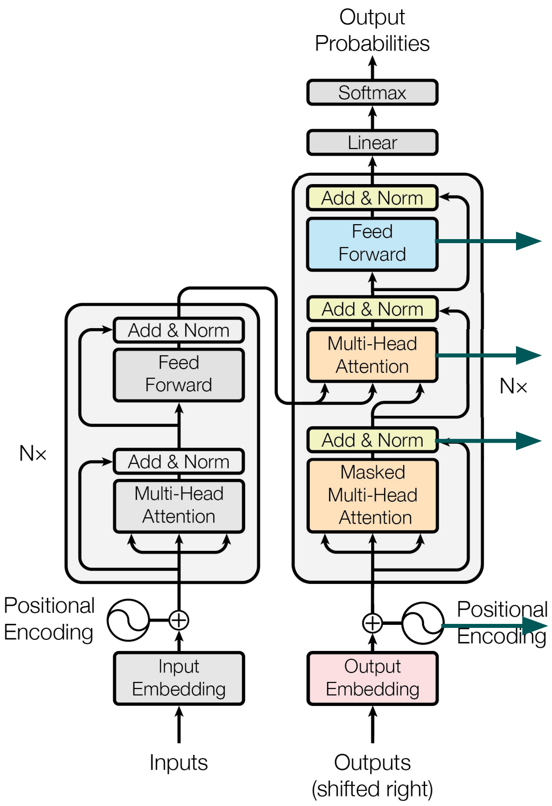
Why?

Places for Improvements



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Positional Encoding: Better Capturing Position Information

Position Encoding: Capturing Position Information

Transformer itself is position agnostic:

$$\text{attention output at position } j = \sum_{i=1}^{T} \text{score}(\mathbf{q}_j, \mathbf{k}_i) \cdot \mathbf{v}_i$$

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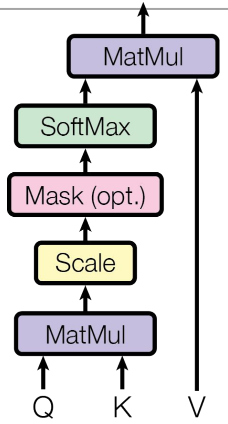

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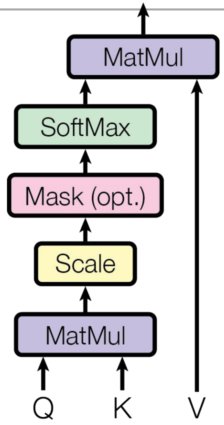
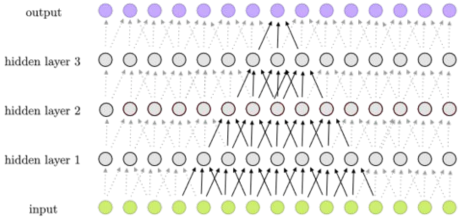


In comparison

CNN has locality prior:



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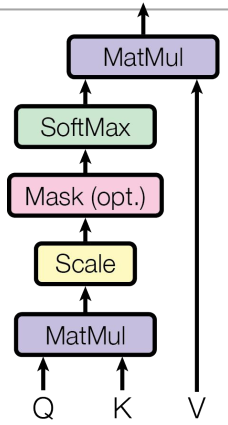

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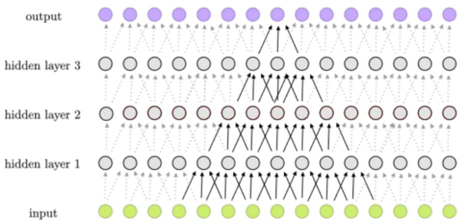

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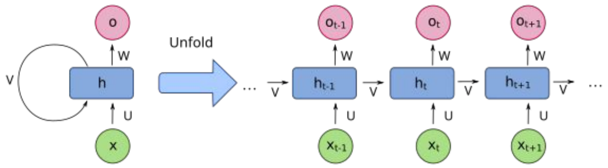

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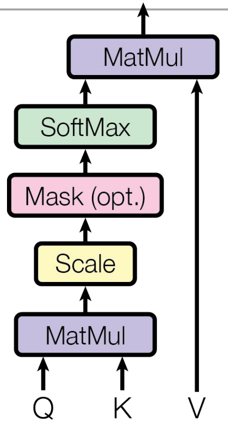

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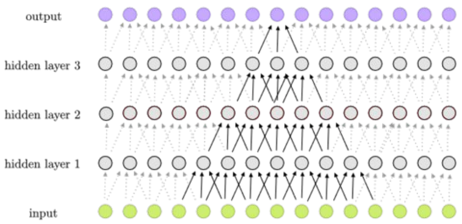

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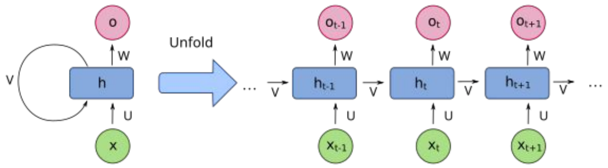

Position encoding adds positional information which is useful for language

Position Encoding: Absolute Position Information

Additive Position Encoding: add the positional information in the token embedding layer

$$\boldsymbol{x}' = \boldsymbol{x} + \underline{\boldsymbol{p}}_{pos}$$

Position Embedding at position pos

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$$p_{pos,2i} = sin(pos/10000^{2i/d})$$
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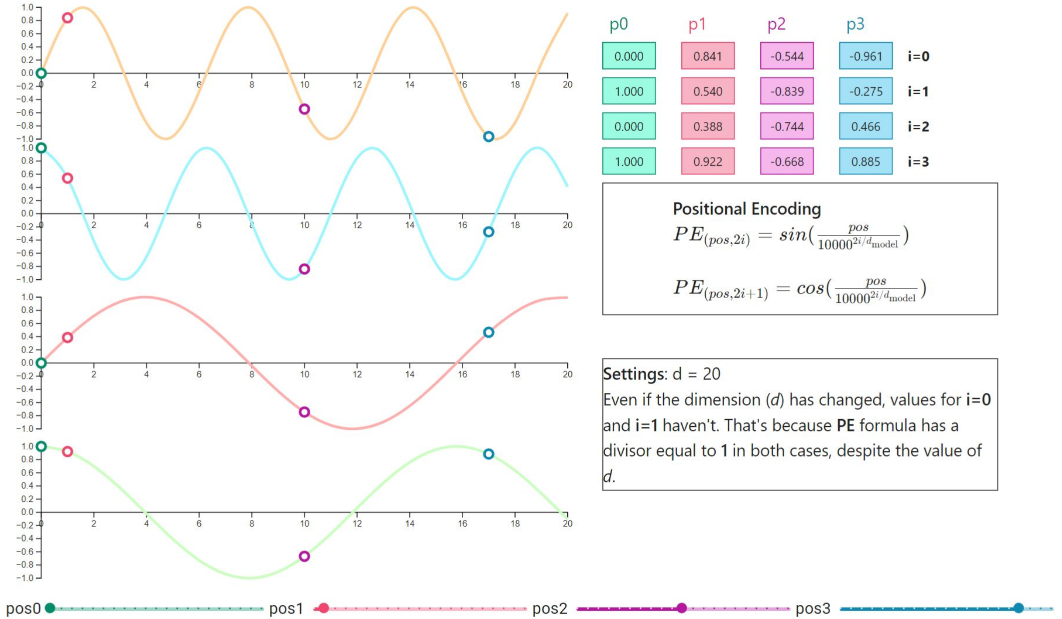

https://erdem.pl/2021/05/understanding-positional-encoding-in-transformers

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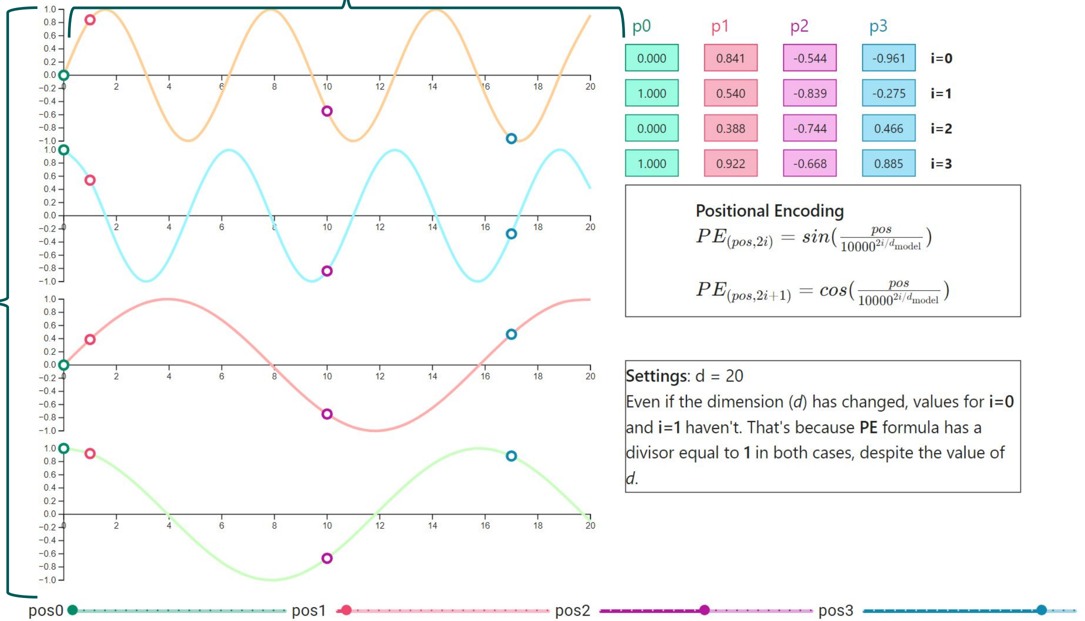
Different wavelength at different embedding dimension to capture different relative positions

Adding different values based on positions



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One embedding vector for each pos

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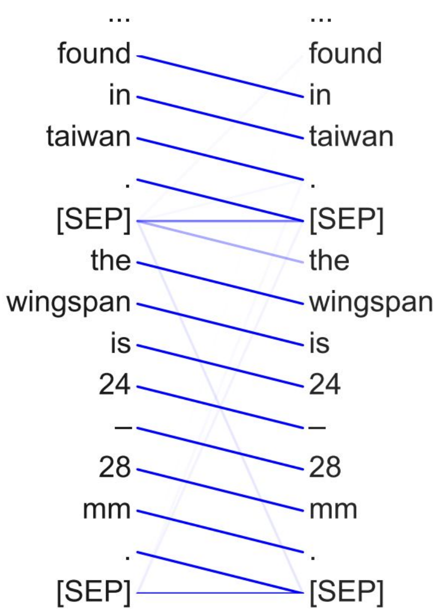

Learned some strong
position-based attention patterns [8]

[8] Clark et al. 2019. What Does BERT Look At? An Analysis of BERT's Attention.

Position Encoding: Relative Position Information

Language Prior: Only relative positions matters in language

I took my dog, Fido, to the park for his walk….

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Blablablabla…I took my dog, Fido, to the park for his walk….

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Trainable Relative Position Bias

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Trainable Relative Position Bias

Model	Position Information	EN-DE BLEU	EN-FR BLEU
Transformer (base)	Absolute Position Representations	26.5	38.2
Transformer (base)	Relative Position Representations	**26.8**	**38.7**
Transformer (big)	Absolute Position Representations	27.9	41.2
Transformer (big)	Relative Position Representations	**29.2**	**41.5**

Performance of Relative Position Embedding on Machine Translation [10]

[9] Raffel et al. 2020. Exploring the limits of transfer learning with a unified text-to-text transformer
[10] Shaw et al. 2018. Self-Attention with Relative Position Representations

Position Encoding: Rotational Position Embedding

Geometry of dot product in attention mechanism

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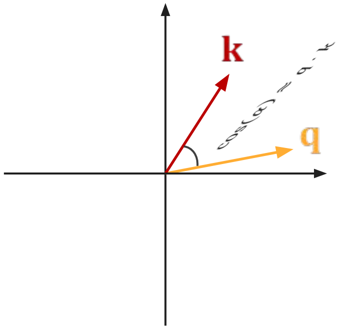

Attention score roughly as cosine of the vectors, assuming unit-lengths.

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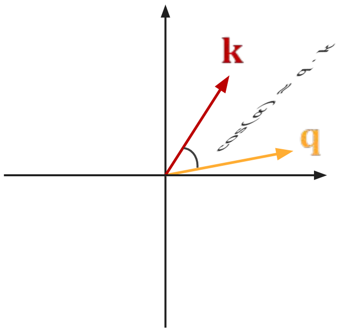

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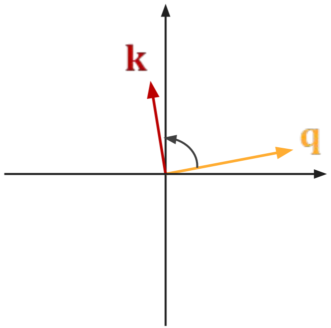

Lower attention importance if positions are far: rotating away

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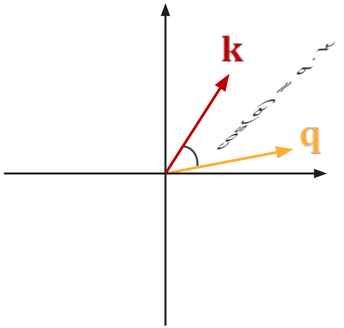

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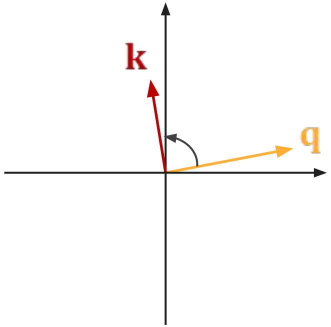

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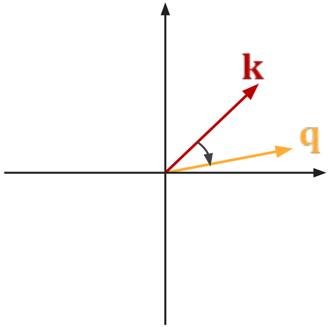

Higher attention importance if positions are close: rotating close

Position Encoding: Rotational Position Embedding

How to make the rotation only depend on relative positions?

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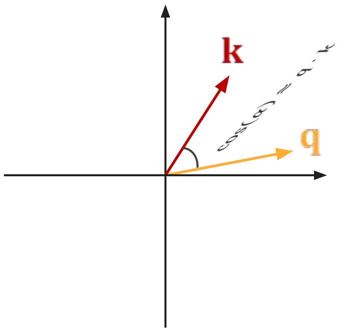

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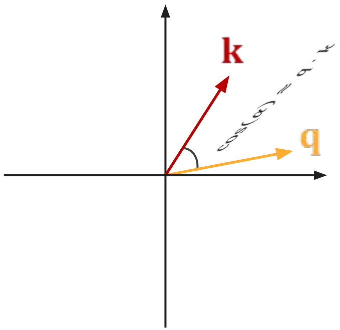

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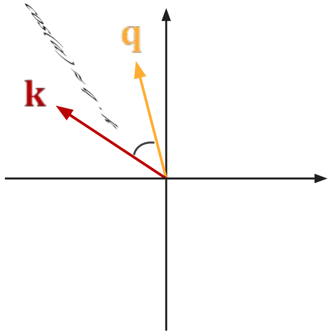
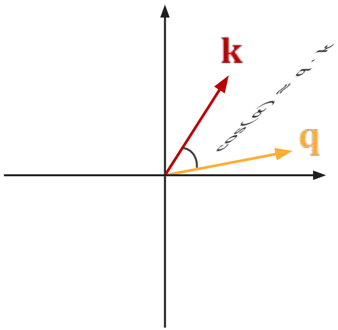


Rotating vectors together for the same disagrees based on positions changes

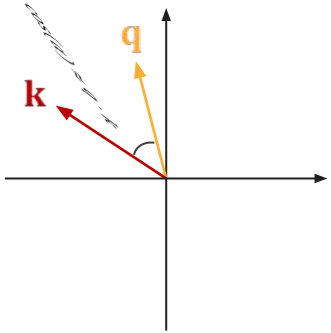
Position Encoding: Rotational Position Embedding

How to make the rotation only depend on relative positions?

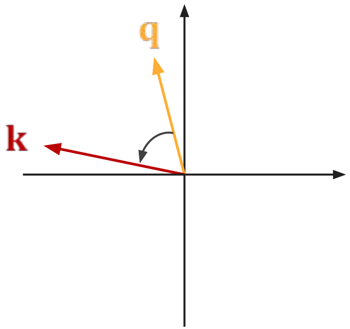
$$\text{Attention score}(\mathbf{q}_j, \mathbf{k}_i) = g(\mathbf{q}_j, \mathbf{k}_i, i - j)$$



Attention score roughly as cosine of the vectors, assuming unit-lengths.



Rotating vectors together for the same disagrees based on positions changes

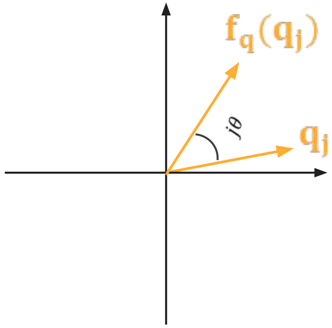


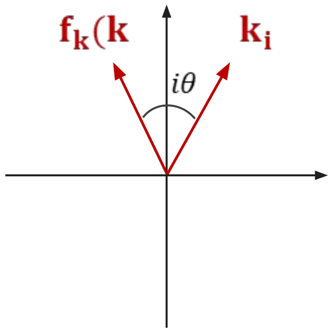
Position based prior holds the same at new absolute positions

Position Encoding: Rotational Position Embedding

Incorporate the vector rotation in the attention mechanism (2d space) [11]:

$$f_q(q_j) = \begin{pmatrix} \cos j\theta & -\sin j\theta \\ \sin j\theta & \cos j\theta \end{pmatrix} \begin{pmatrix} q_j^1 \\ q_j^2 \end{pmatrix} \qquad f_k(k_i) = \begin{pmatrix} \cos i\theta & -\sin i\theta \\ \sin i\theta & \cos i\theta \end{pmatrix} \begin{pmatrix} k_i^1 \\ k_i^2 \end{pmatrix} \qquad \theta_k = (1/10000^{2(i-1)/d})$$





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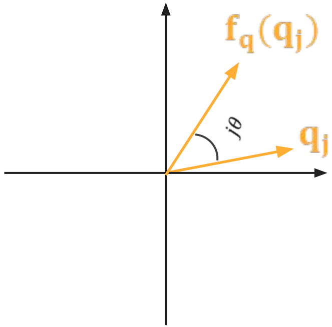
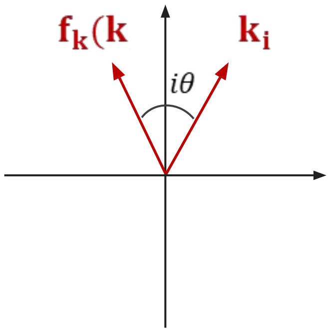
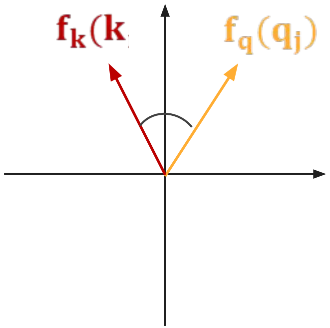


Rotate q by $j\theta$



Rotate k by $i\theta$



Attention only depends on $i - j$

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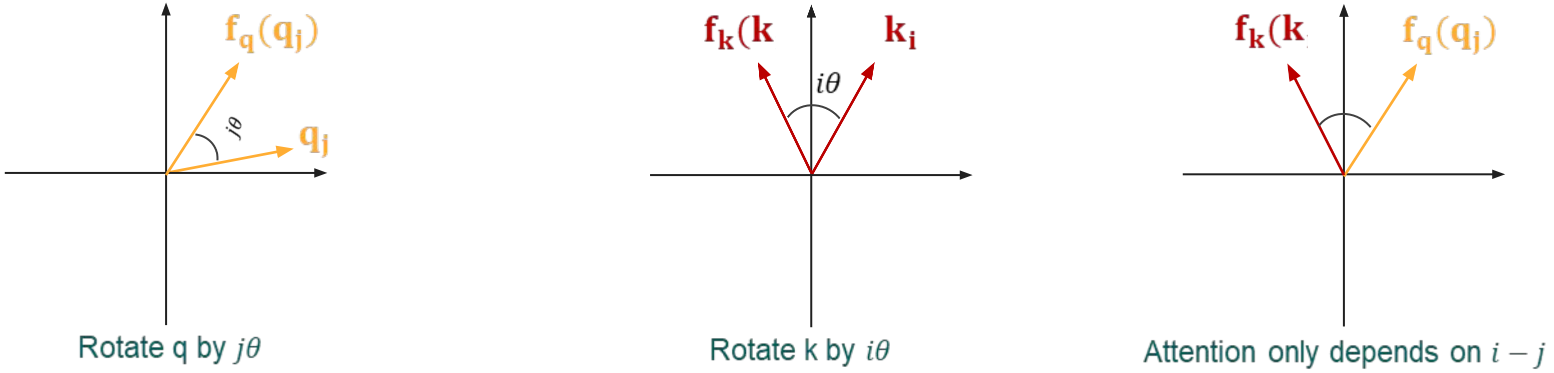

Attention score by the dot prod of rotated vectors:

$$\text{Attention score}(\mathbf{q}_j, \mathbf{k}_i) = f_q(q_j) \cdot f_k(k_i) = \begin{pmatrix} q_j^1 \\ q_j^2 \end{pmatrix}^T \begin{pmatrix} \cos j\theta & -\sin j\theta \\ \sin j\theta & \cos j\theta \end{pmatrix}^T \begin{pmatrix} \cos i\theta & -\sin i\theta \\ \sin i\theta & \cos i\theta \end{pmatrix} \begin{pmatrix} k_i^1 \\ k_i^2 \end{pmatrix}$$

Position Encoding: Rotational Position Embedding

Full form in the high dimensional space [11]:

$$f_{q,k}(x_i) = \begin{pmatrix} \begin{pmatrix} \cos i\theta_1 & -\sin i\theta_1 \\ \sin i\theta_1 & \cos i\theta_1 \end{pmatrix} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \begin{pmatrix} \cos i\theta_{d/2} & -\sin i\theta_{d/2} \\ \sin i\theta_{d/2} & \cos i\theta_{d/2} \end{pmatrix} \end{pmatrix} \begin{matrix} \boxed{\begin{pmatrix} x_i^1 \\ x_i^2 \end{pmatrix}} \\ \vdots \\ \begin{pmatrix} x_i^{d/2} \\ x_i^{d/2} \end{pmatrix} \end{matrix}$$

Partition dimensions into pairs and do the 2d rotation on each pair

With different wavelet lengths: $\theta_k = (1/10000^{2(k-1)/d})$

Position Encoding: Rotational Position Embedding

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Partition dimensions into pairs and do the 2d rotation on each pair

With different wavelet lengths: $\theta_k = (1/10000^{2(k-1)/d})$

Rooted in the sinusoid absolute position embedding, but does multiplication (rotation):

$$\boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{p}_{pos} \qquad p_{pos,2i} = sin(pos/10000^{2i/d})$$
$$p_{pos,2i+1} = cos(pos/10000^{2i/d})$$

"We chose this function because we hypothesized it would allow the model to easily learn to attend by relative positions"---Transformer Paper

[11] Sun et al. 2023. RoFormer: Enhanced transformer with Rotary Position Embedding

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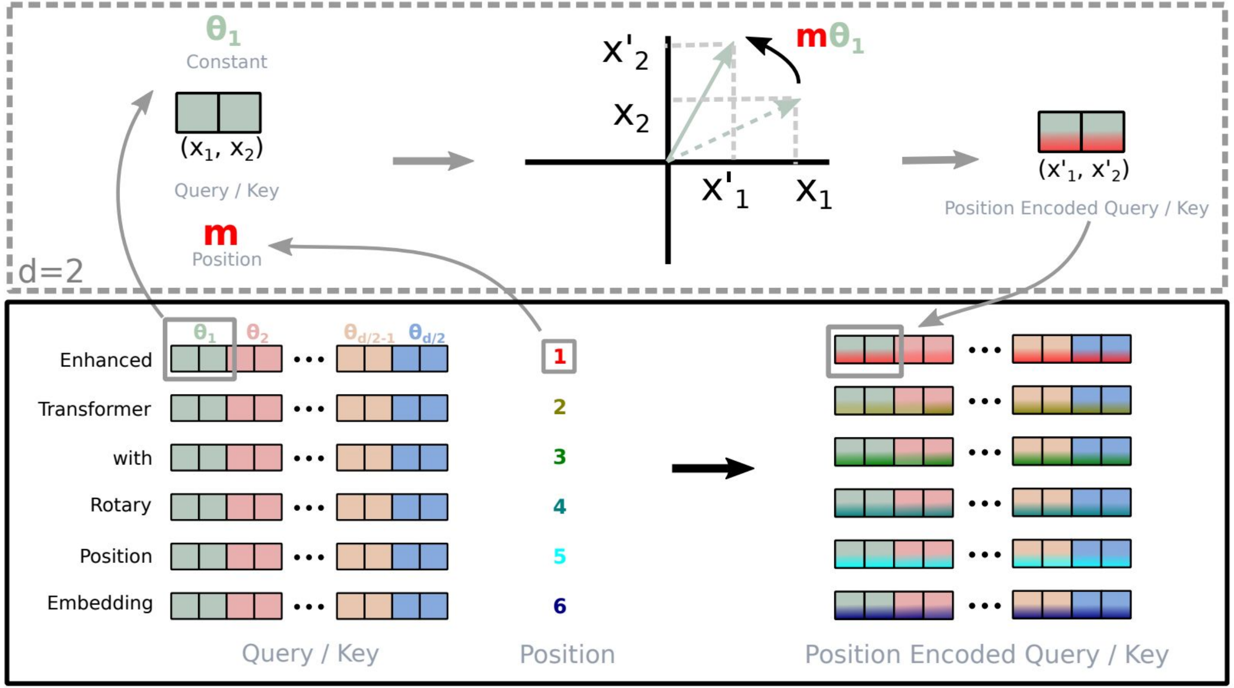
Putting it all together:

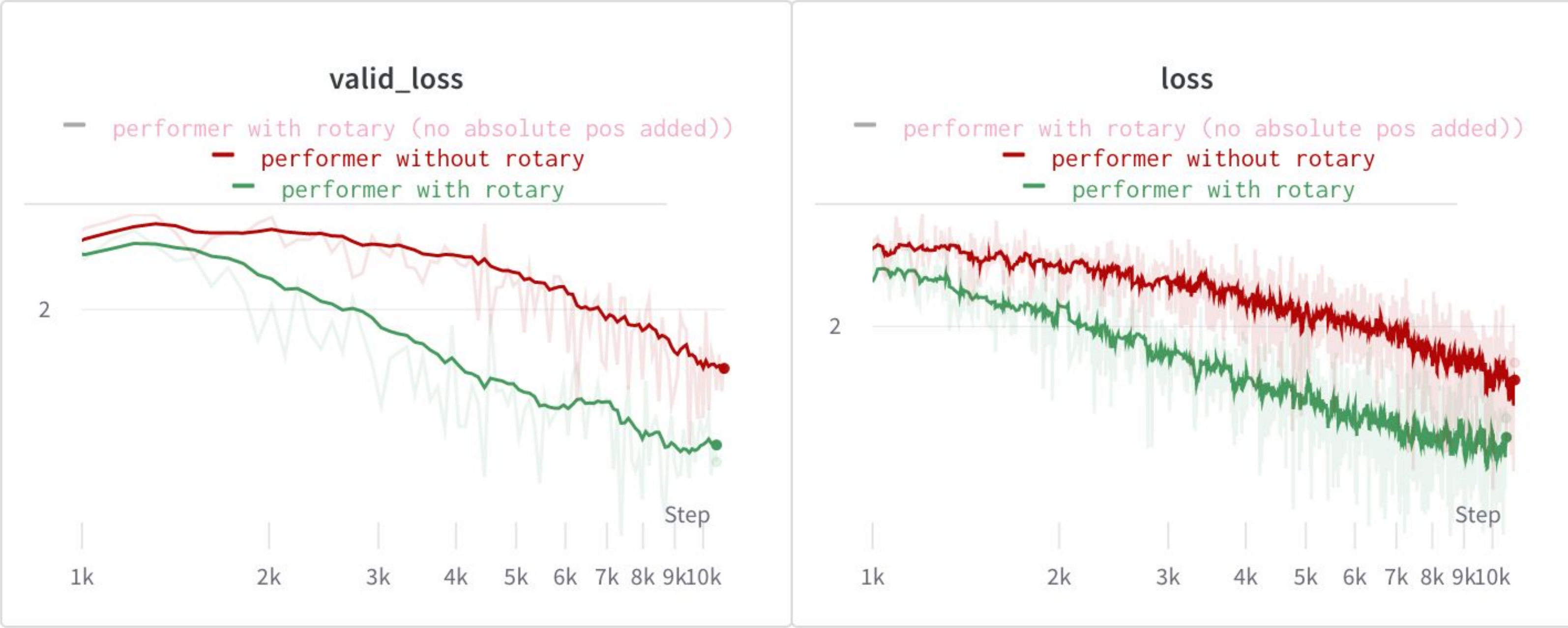


RoPE Embedding [11]

[11] Sun et al. 2023. RoFormer: Enhanced transformer with Rotary Position Embedding

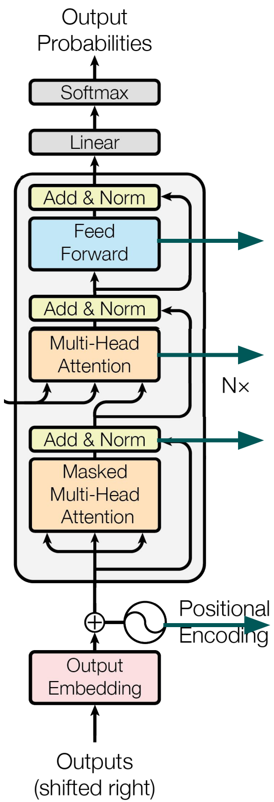
Position Encoding: Rotational Position Embedding

Performance with RoPE



https://blog.eleuther.ai/rotary-embeddings/

LLaMA3's Choice



Feed Forward: SwiGLU

Attention: Grouped-Query Attention

Layer Norm: Pre-Layernorm with RMSNorm

Positional Encoding: RoPE

Questions?