

Scaling ViTs across Training Compute

by Marvin [in](#)

A journey across optimization levels

Looking back at when we could only reliably produce Shakespearean poetry with RNNs, a thin line between hallucinations and poetry, one can see why Google open sourcing Transformers was the just needed *krabby patty secret formula* to SOTA models toppling leaderboards every coming week, and copyright lawsuits enriching the lawyers in the same way that AI ideas could be well thought out as a well pipelined autocomplete service driving some startups. This article is a no exception, *thanks Transformers!*, written from the curiosity that inspires I to sit on the shoulders of giants, intellectually speaking, and start off this chain of optimization across languages and hardware stack that only climaxes limited to the largest GPU compute I can access without feeling like I have leaked my AWS cloud keys to the best crypto miners in the east continents!

Back in time

Vaswani et al. didn't understand the gravity of their research¹ when they lightly ended their paper, but it inspired to generalize learning in the natural language domain, being largely parallelizable and solving saturation in training performance for increased training data.

Recurrent Neural Networks² was the precursor to this, its encoder that generates the latent space representation of the input tokens working in such a way that it captures the entire meaning of the input sentence in its final hidden state. This processing of the entire input text was its drawback as it could not access intermediate hidden states hence not capturing dependencies within words in the sentence.

Sweet sauce of Transformers

Parallelizability, scaled dot product attention, and scaling of models to unprecedented size while maintaining trainability.

¹ [arXiv:1706.03762](#)

Attention is all you need
Vaswani et al. 2017

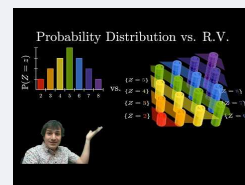
² RNNs can be understood using a special key word, **recurrent**, meaning to recur, where each hidden state would have a loop within itself and also includes the compounded outputs of all the previous hidden states, hugely based on the concept of a Markov model

Markov process is a stochastic process with the properties:

- number of possible states is finite
- outcome at any state depends only on outcomes of previous states
- probabilities are constant over time

where a **stochastic process** can be said as a probability distribution over a space of paths; this path often describing the evolution of some **random variable** over time.

A random variable, despite its name, is never random, and not a variable, it is a deterministic function.



Thanks to Dr Mihai for this awesome video explaining much on this

<https://youtu.be/KQHfOZHnz3k?si=jWPeMLZV0EF76mGz>

From a black box approach

Given a text *The ruler of a kingdom is a* with the next likely word being *king*, humanly thinking, how is the input sentence then passed to a Transformers model?

Basically, computational models cannot process strings, hence it needs conversion to a vector of integers, each word (or subword) uniquely mapped to a corresponding integer, a process known as *tokenization*. A basic form would be a hashmap of words to integers and vice versa for getting a word from index of maximum probability in softmaxed one-dimensional distribution of output float values³.

Implementing a simple tokenizer based on the vocabulary⁴ we have,

```
text = "The ruler of a kingdom is a"
text = text.lower() # making tokenizer case insensitive
text = text.split() # getting individual words
# as separated by spaces
vocab = list(sorted(set(text)))
words_to_ids = {word:i for i, word in enumerate(vocab)}
ids_to_words = {v:k for k,v in words_to_ids.items()}
```

Great, now we have lookup tables (the last two lines), and a naive preprocessing of text needed before tokenization. So then, let's tokenize *the kingdom had another ruler*. Wait?! The lookup table does not have the words "*another*", "*had*", "*another*"! Let's improve it so any word not part of the original vocabulary be assigned a new unique id⁵.

```
words_to_ids = {word:i for i, word in enumerate(vocab)}
ids_to_words = {v:k for k,v in words_to_ids.items()}
def lookup(word):
    try:
        id = words_to_ids[word]
    except KeyError:
        vocab.append(word)
        words_to_ids[word] = len(vocab) - 1
        ids_to_words[len(vocab)-1] = word
        id = words_to_ids[word]
    return id
```

³ the commonly used tokenizer is tiktoken, using a concept called Byte-Pair Encoding to map subwords to ids using a look-up table that takes into account frequencies of subwords.

⁴ vocabulary ~ set of unique words (or subwords based on the tokenization strategy) in all words of the entire training dataset used to train a particular large language model.

⁵ our look-up tables are very much capable of any encoding and decoding (for the tiny vocabulary).

Trying our shiny code

```
sentence = "the kingdom had another ruler"
tokens = [lookup(word) for word in
          sentence.lower().split()]
print(tokens)
# [5, 2, 6, 7, 4]
words_gotten = [ids_to_words[id] for id in tokens]
sentence_gotten = " ".join(words_gotten)
print(sentence_gotten)
# "the kingdom had another ruler"
```

Note that the above implementation of tokenization is to help you understand a baseline of what happens under the hood in conversion of what models cannot deal with, strings, to a format that can be computationally crunched.

However, when looking into the Transformers model architecture as outlined in the paper¹, also in⁶ for convenience, it is seen that the first block is an Embedding block.

What about the Embeddings block?

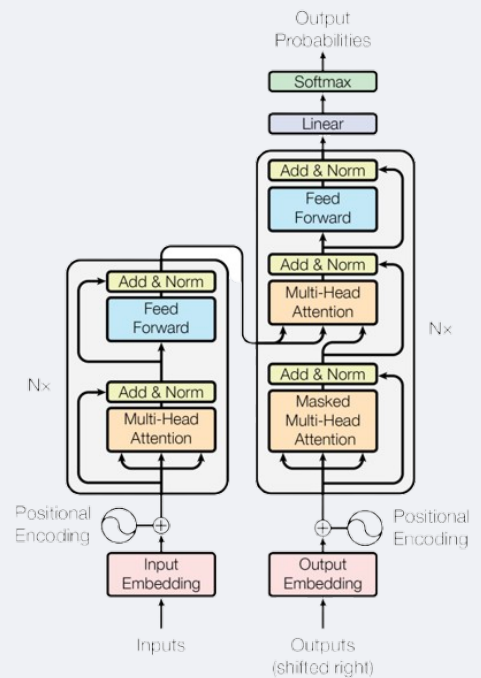
Well, the vector of integers as input in itself cannot capture rich latent representations of the input tokens, so the Embeddings block⁷ does just that, mapping the tokens to higher dimensions. The embeddings block is usually V by D , where V is the size of the vocabulary, and D is an abstract dimension of your choosing, the higher the better, but more computationally expensive and longer to process.

Using PyTorch, an Embeddings block of D being 3 can be implemented as:

```
import torch, torch.nn as nn
V, D = len(vocab), 3
emb = nn.Embedding(V,D)
higher_emb_tokens = emb(torch.tensor(tokens))
print(higher_emb_tokens.shape) # torch.Size([5, 3])
```

One of the best LLMs ever open sourced by Meta, the Llama 3, the 3 billion parameter size variant, has its vocabulary with 128K tokens. and the embedding dimensions, D , being 3072.

⁶ Transformers architecture



⁷ `nn.Embedding` is just `nn.Linear` but only that `nn.Embedding` simplifies retrieving rows from its weights such that you don't pass it one-hot vectors but just indices basically same as the position of the single 1s in the one-hot vector you would have passed to `nn.Linear`

Positional Encoding

Before the Multi-Head Attention (MHA) block, the positional encoding is attached to the graph to constitute the position information and this allows the model to easily attend to relative positions. Why is that? Well, the MHA block is permutation-equivariant, and cannot distinguish whether an input comes before another one in the sequence or not.

The meaning of a sentence can change if words are reordered, so this technique retains information about the order of the words in a sequence.

Positional encoding is the scheme through which the knowledge of the order of objects in a sequence is maintained.

This post by Christopher⁸ highlights the evolution of positional encoding in transformer models, a worthy read! For this article, let's focus on the rotary positional embedding (RoPE)⁹.

Let's making a few things clear,

- previous position encodings were done before the MHA block, this is done within it.
- RoPE are only applied to the queries and the keys, not the values.
- RoPE are only applied after the vectors \vec{q} and \vec{k} have been multiplied by the W matrix in the attention mechanism, while in the vanilla transformer they're applied before.

The general form of the proposed approach for RoPE is as in page 5 for a sparse matrix with pre-defined parameters

$$\Theta = \{\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, \dots, d/2]\}$$

which can be implemented in code as

```
assert d % 2 == 0, "dim must be divisible by 2"
i_s = torch.arange(0,d,2).float()
theta_s = 10000 ** (- i_s / d).to(device)
```

where *device* is code that chooses the compute device.

```
device = torch.device(
    "cuda" if torch.cuda.is_available() else (
        "mps" if torch.backends.mps.is_available() else "cpu"
    )
)
```

⁸ <https://huggingface.co/blog/designing-positional-encoding>

You could have designed state of the art positional encoding
Christopher Fleetwood

⁹ [arXiv:2104.09864](https://arxiv.org/abs/2104.09864)

RoFormer: Enhanced Transformer with Rotary Position Embedding
Su et al. 2022

Given the computational efficient realization which is what we're aiming at getting

¹⁰ `context_len` is an integer which refers to the maximum number of tokens the model can consider in a single forward pass

$$R_{\Theta, m}^d \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{d-1} \\ x_d \end{pmatrix} \otimes \begin{pmatrix} \cos m\theta_1 \\ \cos m\theta_1 \\ \cos m\theta_2 \\ \cos m\theta_2 \\ \vdots \\ \cos m\theta_{d/2} \\ \cos m\theta_{d/2} \end{pmatrix} + \begin{pmatrix} -x_2 \\ x_1 \\ -x_4 \\ x_3 \\ \vdots \\ -x_d \\ x_{d-1} \end{pmatrix} \otimes \begin{pmatrix} \sin m\theta_1 \\ \sin m\theta_1 \\ \sin m\theta_2 \\ \sin m\theta_2 \\ \vdots \\ \sin m\theta_{d/2} \\ \sin m\theta_{d/2} \end{pmatrix}$$

Having implemented $\vec{\theta}$, next let's implement $m\vec{\theta}$ by way of an outer product¹⁰

```
m = torch.arange(context_len, device=device)
freqs = torch.outer(m, theta_s).float()
```

$$m\vec{\theta} = \text{freqs} = \begin{pmatrix} m_1\theta_1, m_1\theta_2, \dots, m_1\theta_{d/2-1}, m_1\theta_{d/2} \\ m_2\theta_1, m_2\theta_2, \dots, m_2\theta_{d/2-1}, m_2\theta_{d/2} \\ \vdots \quad \vdots \quad \dots \quad \vdots \quad \vdots \\ m_{\text{ctx_len}}\theta_1, m_{\text{ctx_len}}\theta_2, \dots, m_{\text{ctx_len}}\theta_{d/2-1}, m_{\text{ctx_len}}\theta_{d/2} \end{pmatrix}$$

It is then needed to get the complex numbers for the resulting matrix of size context len by $d/2$.

```
freqs_complex = torch.polar(torch.ones_like(freqs), freqs)
```

which then gives the polar form of each element in the matrix, such that

$$e^{im\vec{\theta}} = \begin{pmatrix} \cos(m_1\theta_1) + i \sin(m_1\theta_1), \cos(m_1\theta_2) + i \sin(m_1\theta_2), \dots, \cos(m_1\theta_{d/2}) + i \sin(m_1\theta_{d/2}) \\ \cos(m_2\theta_1) + i \sin(m_2\theta_1), \cos(m_2\theta_2) + i \sin(m_2\theta_2), \dots, \cos(m_2\theta_{d/2}) + i \sin(m_2\theta_{d/2}) \\ \vdots \quad \quad \quad \vdots \quad \quad \quad \dots \quad \quad \quad \vdots \quad \quad \quad \vdots \\ \cos(m_{cl}\theta_1) + i \sin(m_{cl}\theta_1), \cos(m_{cl}\theta_2) + i \sin(m_{cl}\theta_2), \dots, \cos(m_{cl}\theta_{d/2}) + i \sin(m_{cl}\theta_{d/2}) \end{pmatrix}$$

Let's consider a subset of the inputs and a subset of the matrix above, then

$$\begin{aligned} \vec{x} &= \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \end{pmatrix} = \begin{pmatrix} x_1 + ix_2 \\ x_3 + ix_4 \end{pmatrix} \otimes \begin{pmatrix} f_{11} + i\hat{f}_{11} \\ f_{12} + i\hat{f}_{12} \end{pmatrix}, \text{ where } \begin{cases} f_{11} = \cos(m_1\theta_1) \\ \hat{f}_{11} = \sin(m_1\theta_1) \\ f_{12} = \cos(m_1\theta_2) \\ \hat{f}_{12} = \sin(m_1\theta_2) \end{cases} \\ &= (x_1 + ix_2)(f_{11} + i\hat{f}_{11}) = x_1f_{11} - x_2\hat{f}_{11} + i(x_1\hat{f}_{11} + x_2f_{11}) \\ &\quad \text{meaning } \begin{pmatrix} x_1 + ix_2 \\ x_3 + ix_4 \end{pmatrix} \otimes \begin{pmatrix} f_{11} + i\hat{f}_{11} \\ f_{12} + i\hat{f}_{12} \end{pmatrix} \\ &= \begin{pmatrix} x_1f_{11} - x_2\hat{f}_{11} + i(x_1\hat{f}_{11} + x_2f_{11}) \\ x_3f_{12} - x_4\hat{f}_{12} + i(x_3\hat{f}_{12} + x_4f_{12}) \end{pmatrix} = \begin{pmatrix} x_1f_{11} - x_2\hat{f}_{11} & x_1\hat{f}_{11} + x_2f_{11} \\ x_3f_{12} - x_4\hat{f}_{12} & x_3\hat{f}_{12} + x_4f_{12} \end{pmatrix} \\ &\quad \text{rearranging gives} \\ &= \begin{pmatrix} x_1f_{11} - x_2\hat{f}_{11} \\ x_1\hat{f}_{11} + x_2f_{11} \\ x_3f_{12} - x_4\hat{f}_{12} \\ x_3\hat{f}_{12} + x_4f_{12} \end{pmatrix} \Rightarrow \begin{pmatrix} x_1 \cos m_1\theta_1 - x_2 \sin m_1\theta_1 \\ x_1 \sin m_1\theta_1 + x_2 \cos m_1\theta_1 \\ x_3 \cos m_1\theta_2 - x_4 \sin m_1\theta_2 \\ x_3 \sin m_1\theta_2 + x_4 \cos m_1\theta_2 \end{pmatrix} \end{aligned}$$

Implementing the rotation mechanism

the previously derived mathematical algorithm can then be translated into code as below.

```
def apply_rotary_embs(x, freqs_complex, device):
    # x rearrange and make complex => result => x1 + jx2
    # [B, context_len, H, head_dim] => [B, context_len, H, head_dim/2]
    x_c = torch.view_as_complex(
        x.float().reshape(*x.shape[:-1], -1, 2)
    )
    # [context_len, head_dim/2] => [1, context_len, 1, head_dim/2]
    f_c = freqs_complex.unsqueeze(0).unsqueeze(2)
    # [B, context_len, H, head_dim/2] * [1, context_len, 1, head_dim/2]
    # => [B, context_len, H, head_dim/2]
    x_rotated = x_c * f_c
    # [B, context_len, H, head_dim/2] => [B, context_len, H,
        head_dim/2, 2]
    x_out = torch.view_as_real(x_rotated)
    # [B, context_len, H, head_dim/2, 2] => [B, context_len, H,
        head_dim]
    x_out = x_out.reshape(*x.shape)
    return x_out.type_as(x).to(device)
```

And now to the most interesting part of this architecture....

Multi-Head Attention¹³

a picture is worth a thousand words! Let it do the talking!

¹¹ `nn.Linear` is an instance initialization of a stack of perceptrons in a single layer in PyTorch, with `d_in` previously known as the abstract dim of the word embedding, and `d_out` is initialized as `d_in`

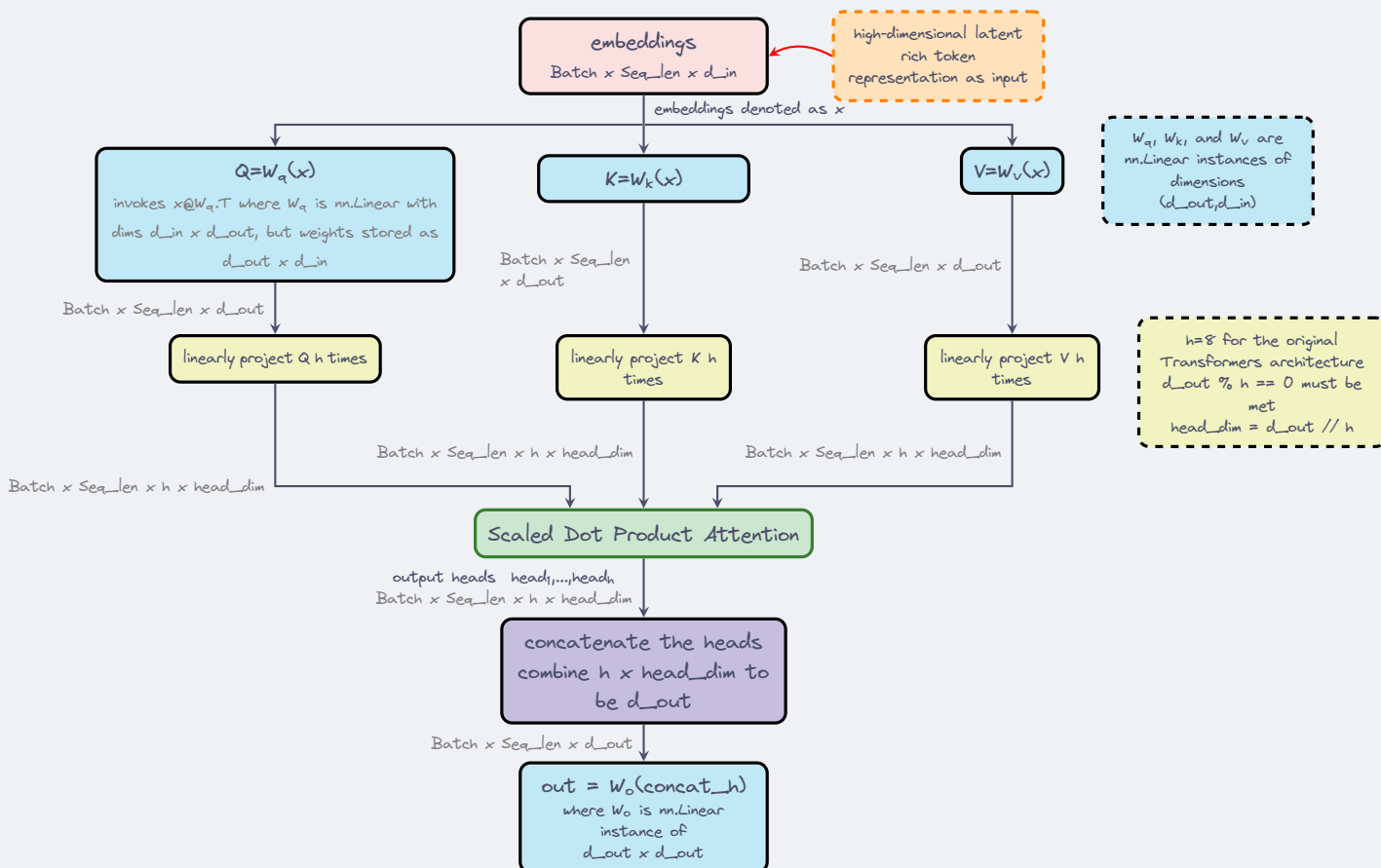
¹² proving the invocation that initializes Q, K and V matrices

```
import torch
import torch.nn as nn
x = torch.randn(10, 3)
Wq = torch.nn.Linear(3, 40, bias=False)
torch.equal(Wq(x), x.dot(Wq.weight.T))
torch.equal(Wq(x), x@Wq.weight.T) # True
```

¹³ the MHA has its core in attention mechanism whose goal is to dynamically decide on which inputs we want to “attend” more than others based on

- *query* ~ a feature vector that describes what we are looking for in the sequence, i.e. what would we maybe want to pay attention to.
- *keys* ~ for each input element, we have a key which is again a feature vector. This feature vector roughly describes what the element is “offering”, or when it might be important. The keys should be designed such that we can identify the elements we want to pay attention to based on the query.

...



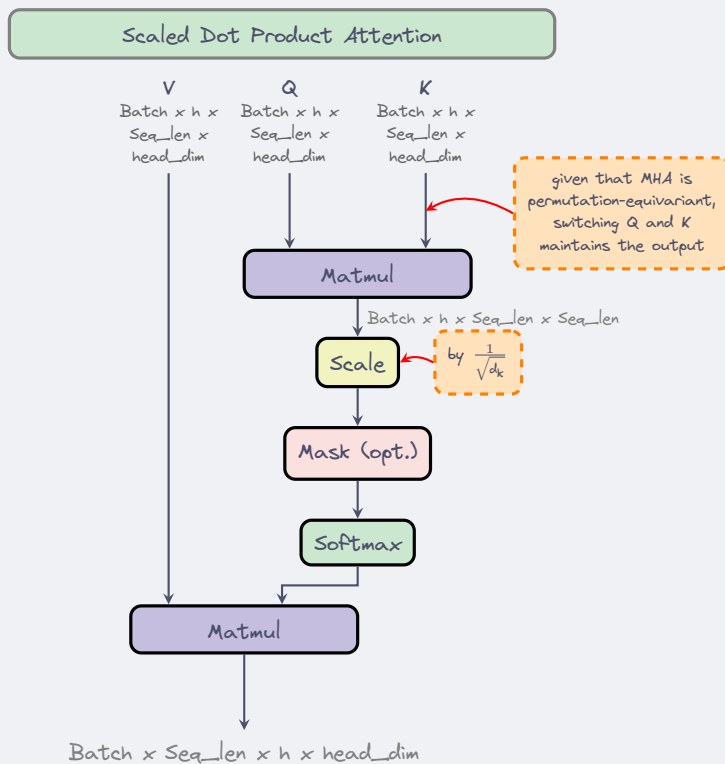
Scaled dot product attention

The term, first introduced in the *Vaswani et al.* paper, involves the following key operations:

- compute the dot product of queries and keys of dimension d_k , QK^T
- scaling by a factor $1/\sqrt{d_k}$ to counteract the effect of extremely small gradients in the softmax computation as will be seen in the next step when d_k becomes very large¹⁴. This begets the attention scores.
- softmax computation of the normalized result attention scores. The result is the attention weights.
- dot product of the attention weights and the values.

the infamous equation is therefore

$$\text{attention}(Q, K, V) = \text{softmax} \left(\frac{QK^T}{\sqrt{d_k}} \right) V$$



From the diagram above, there's a new block, **Mask**, that does something called masking. A transformer usually has two phases, encoding phase and the decoding phase. From the Transformers architecture diagram, encoder is on the left and the decoder on the right for the two phases.

from previous¹³...

- **values** \sim for each input element, we also have a value vector. This feature vector is the one we want to average over.
- **score function** \sim to rate which elements we want to pay attention to, we need to specify a score function. The score function takes the query and a key as input, and outputs the score (attention weight) of the query-key pair. It is usually implemented by simple similarity metrics like a dot product, or a small MLP.



courtesy of [UvA course notes](#)

¹⁴ d_k is the size of the last dimension of the keys after linear projection and transpose, to be implemented later. It is the head dimension for each attention head. Sanity check states that your key dimension be $B \times \text{Seq_len} \times h \times \text{head_dim}$ before this step where d_k is gotten by $k.\text{shape}[-1]$

During the decoding phase, at each step of predicting a word¹⁵, the network needs take a look at the words previous to that step, and output a softmax prediction for what it thinks the next word is. Since transformers attend to the entire sequence, before and after, it becomes a trivial task to predict the next word, simply by putting 100% attention to the word after it.

This of course is cheating, it won't learn anything really. During the inference pipeline, the entire sequence won't be present, hence why we need the masking block, we don't want each word in the decoder to see the words that come after it.

Implementing masking in code

Let's use the sequence below

Eiffel Tower is in Paris

and consider the llama 2 tokenizer¹⁶, *sentencepiece*, as the final Transformers model built on these progressive learnings while building on the architecture is Llama 2.

```
import sentencepiece as spm
sequence = "Eiffel Tower is in Paris"
sp = spm.SentencePieceProcessor("llama-2-7b-tok.model")
tokens = sp.encode_as_ids(sequence)
```

Considering V and D used for *Llama2 model 7B* variant, let's initialize an embedding instance.

```
V, D=32_000, 4_096
emb = nn.Embedding(V, D)
emb_tokens = emb(torch.tensor(tokens))
print(emb_tokens.shape)
# torch.Size([7, 4096])
```

Our embeddings output being the input to scaled dot product attention, let's compute QK^T then scale keeping in mind that the batch dimension, multiple heads, and the positional encoding is not incorporated for the sake of focusing on masking.

```
Wq, Wk, Wv = nn.Linear(D,D), nn.Linear(D,D), nn.Linear(D,D)
q, k, v = Wq(emb_tokens), Wk(emb_tokens), Wv(emb_tokens)
scores=q@k.T
scaled_scores=scores/k.shape[-1]**.5
print(scaled_scores.shape) # torch.Size([7, 7])
```

¹⁵ the model actually predicts a token which, by using a lookup table, is decoded to a word which is what humans understand.

¹⁶ the lookup-table *tokenizer.model* can be found from the huggingface model card for *Llama-2-7b*
<https://huggingface.co/meta-llama/Llama-2-7b/tree/main>


```

torch.set_printoptions(precision=5, sci_mode=False, linewidth=500)
print(scaled_scores)
tensor([[ -0.10457,  -0.23802,   0.08053,   0.33000,  -0.10408,   0.55068,   0.68916],
        [ -0.35013,  -0.04846,   0.65688,   0.18756,  -0.81784,   0.10682,  -0.74313],
        [ -0.26961,  -0.70423,   0.94224,   0.16090,  -0.20169,   0.15549,  -0.28134],
        [ -0.32253,   0.56740,   0.08793,  -0.53429,  -0.19362,  -0.22245,  -0.38808],
        [  0.32020,   0.29380,   0.18501,  -0.53281,   0.02592,  -0.57664,   0.17737],
        [  0.00706,  -0.08485,  -0.11895,   0.21021,   0.50643,   0.48187,   0.11625],
        [  0.38275,   0.45847,  -0.34459,  -0.12443,   0.35930,   0.65530,   0.03805]])
grad_fn=<DivBackward0>

```

Now onto a mask with ones from the first upper off-diagonal onwards. Then, fill them with $-\infty$ such that the exponential of those values will be zero in the weights.

```

mask = torch.triu(torch.ones_like(scaled_scores),
                  diagonal=1)
scaled_scores_masked =
    scaled_scores.masked_fill_(mask.bool(), -torch.inf)
weights = torch.softmax(scaled_scores_masked, dim=-1)

```

Now, for the weights, pre-matrix multiply with V for the result of Scaled Dot Product Attention

```

out = weights @ v
print(out.shape) # torch.Size([7, 4096])

```

Nice! Now onto *Add & Norm* layer, which from the paper, is a Layer normalization that computes

$$\text{LayerNorm}(x + \text{Multihead}(x, x, x))$$

where x is basically the same sequence (as an embedding) input to the $Q, K \& V$. This layer hence is a residual connection necessary for enabling smooth gradient flow through the model and retaining information from the original sequence prior to the multi-head attention. This is simply implemented as

```

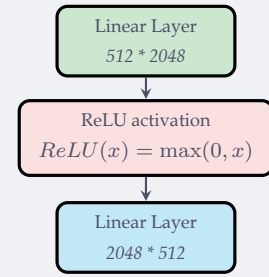
out_attn = multiheadAttn(x)
out = x + out_attn
norm_out = norm(out)

```

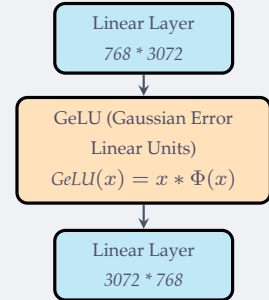
What about the Feed Forward NN layer

Always forming a crucial layer in most models, the FFN, in this case, maps context rich vectors onto a higher dimension¹⁷ which increases learning so it can model more complex relationships and also adds an activation function to introduce non-linear, even better relations.

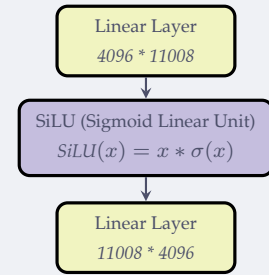
¹⁷ Feed Forward NN layer for Transformer model



Feed Forward NN layer for GPT-2



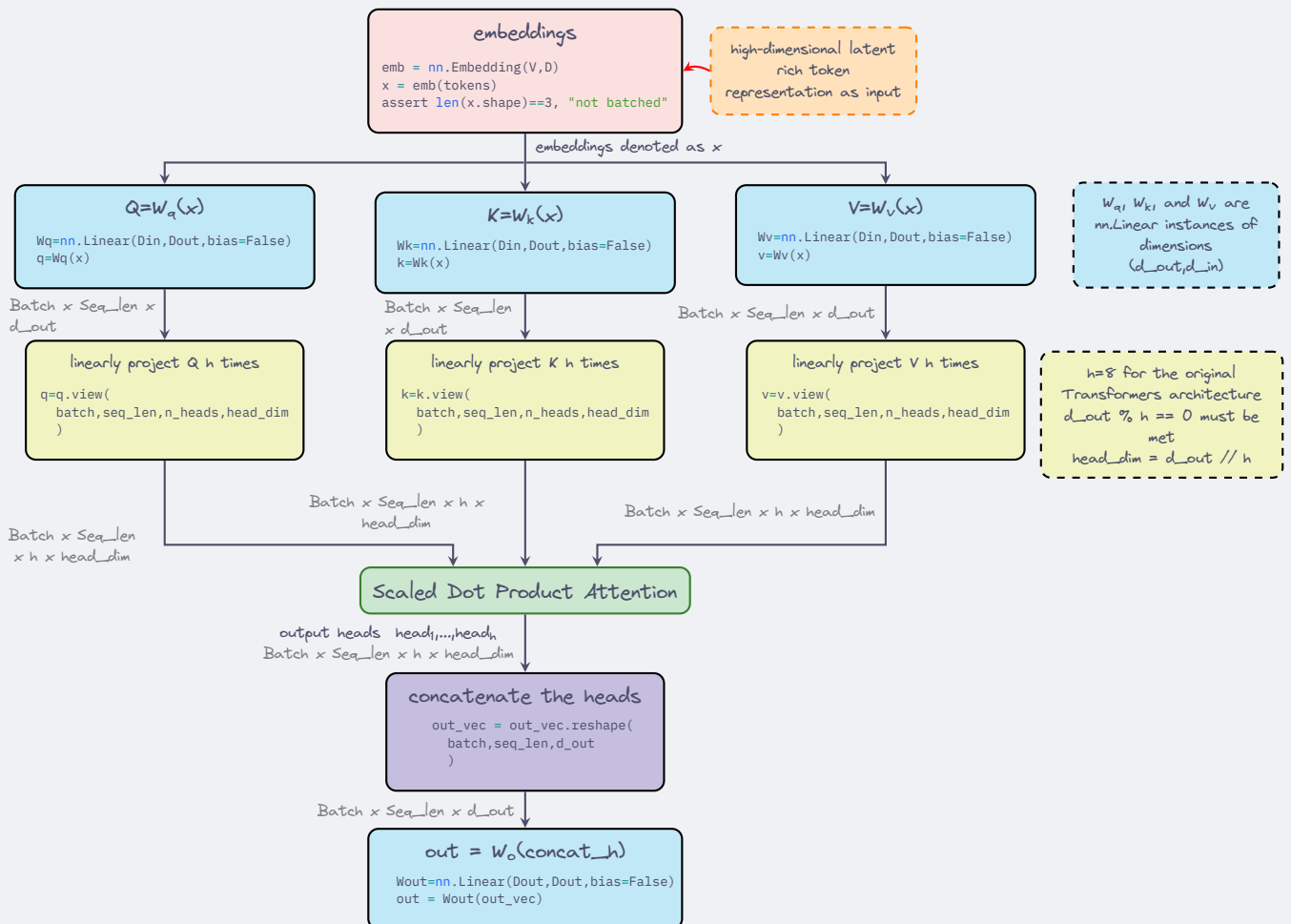
Feed Forward NN layer for Llama-2-7b



Building Llama-2 from the SDPA outwards...

Gladly having gone through the layers in the Transformer model, it is of essence to build the Llama-2 model graph and load the weights for the 7B variant. It is a decoder-only architecture, as is most State of The Art common LLMs. Why is that? Well, decoder-only architectures worked very well for next token prediction and translation tasks, and were easier to train. And so, they picked up as the *de facto* baselines for most current outstanding models.

Earlier, we had the graph for the Multi-head Attention, let's add codes to it to map it to implementation.



NEW PAGE PENDING

lorem ipsum