Scaling ViTs across Training Compute

by Marvin Mboya

A journey across optimization levels

Looking back at when I 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 research[1] 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 Networks[2] 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 hiddetn 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

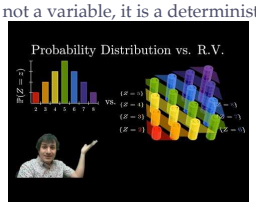
[2] RNNs can be understood using a special key word, **recurrent**, meaning to recur, where each hidden state would have a loop within itself and also includes the compounded outputs of all the previous hidden states, hugely based on the concept of a Markov model

Markov process is a stochastic process with the properties:

- number of posssible states is finite
- outcome at any state depends only on outcomes pf 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 values [3].

Implementing a simple tokenizer based on the vocabulary[4] I 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 I 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 id[5].

```
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] the look-up table is very much capable of any encoding and decoding (for the tiny tiny vocabulary).

Trying the new 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.
Hoever, when looking into the Transformers model architecture as outlined in the paper[1], also in[6] for convenience, it is seen that the first block is an Embedding block.

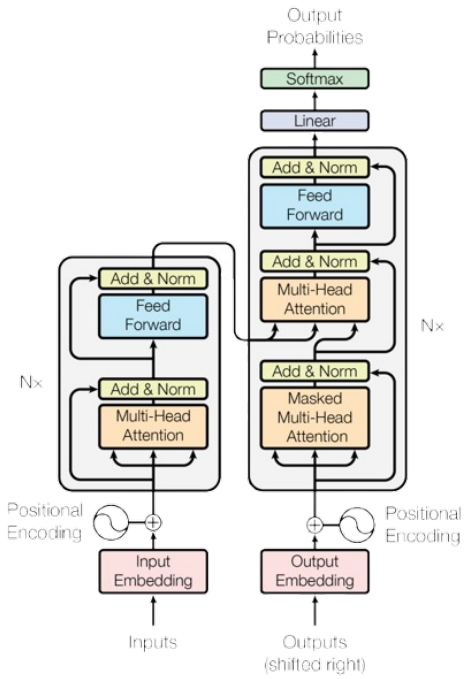
What about the Embeddings block?

Well, the vector of integers as input in itself cannot capture rich latent representations of the input tokens, so the Embeddings block[7] 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 indeces 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 Christopher[8] 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 is only applied to the queries and the keys, not the values.
- RoPE is only applied after the vectors $\vec{q}$ and $\vec{k}$ have been multiplied by the $\boldsymbol{W}$ 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 $\Theta = \{\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, ..., d/2]\}$

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

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

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

Having implemented $\vec{\theta}$, next let's implement $m\vec{\theta}$ by way of an outer product[10]

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

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

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

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

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

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} (x_1 & x_2) \\ (x_3 & x_4) \end{pmatrix} = \begin{pmatrix} x_1 + ix_2 \\ x_3 + ix_4 \end{pmatrix} \otimes \begin{pmatrix} f_{11} + i\hat{f}_{11} \\ f_{12} + i\hat{f}_{12} \end{pmatrix}, \text{ where } \begin{cases} f_{11} = \cos(m_1\theta_1) \\ \hat{f}_{11} = \sin(m_1\theta_1) \\ f_{12} = \cos(m_1\theta_2) \\ \hat{f}_{12} = \sin(m_1\theta_2) \end{cases}$$

$$= (x_1 + ix_2)(f_{11} + i\hat{f}_{11}) = x_1f_{11} - x_2\hat{f}_{11} + i(x_1\hat{f}_{11} + x_2f_{11})$$

meaning $\begin{pmatrix} x_1 + ix_2 \\ x_3 + ix_4 \end{pmatrix} \otimes \begin{pmatrix} f_{11} + i\hat{f}_{11} \\ f_{12} + i\hat{f}_{12} \end{pmatrix}$

$$= \begin{pmatrix} x_1f_{11} - x_2\hat{f}_{11} + i(x_1\hat{f}_{11} + x_2f_{11}) \\ x_3f_{12} - x_4\hat{f}_{12} + i(x_3\hat{f}_{12} + x_4f_{12}) \end{pmatrix} = \begin{pmatrix} (x_1f_{11} - x_2\hat{f}_{11} & x_1\hat{f}_{11} + x_2f_{11}) \\ (x_3f_{12} - x_4\hat{f}_{12} & x_3\hat{f}_{12} + x_4f_{12}) \end{pmatrix}$$

rearranging gives

$$= \begin{pmatrix} x_1f_{11} - x_2\hat{f}_{11} \\ x_1\hat{f}_{11} + x_2f_{11} \\ x_3f_{12} - x_4\hat{f}_{12} \\ x_3\hat{f}_{12} + x_4f_{12} \end{pmatrix} \Rightarrow \begin{pmatrix} x_1\cos m_1\theta_1 - x_2\sin m_1\theta_1 \\ x_1\sin m_1\theta_1 + x_2\cos m_1\theta_1 \\ x_3\cos m_1\theta_2 - x_4\sin m_1\theta_2 \\ x_3\sin m_1\theta_2 + x_4\cos m_1\theta_2 \end{pmatrix}$$

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

Implementing the rotation mechanism

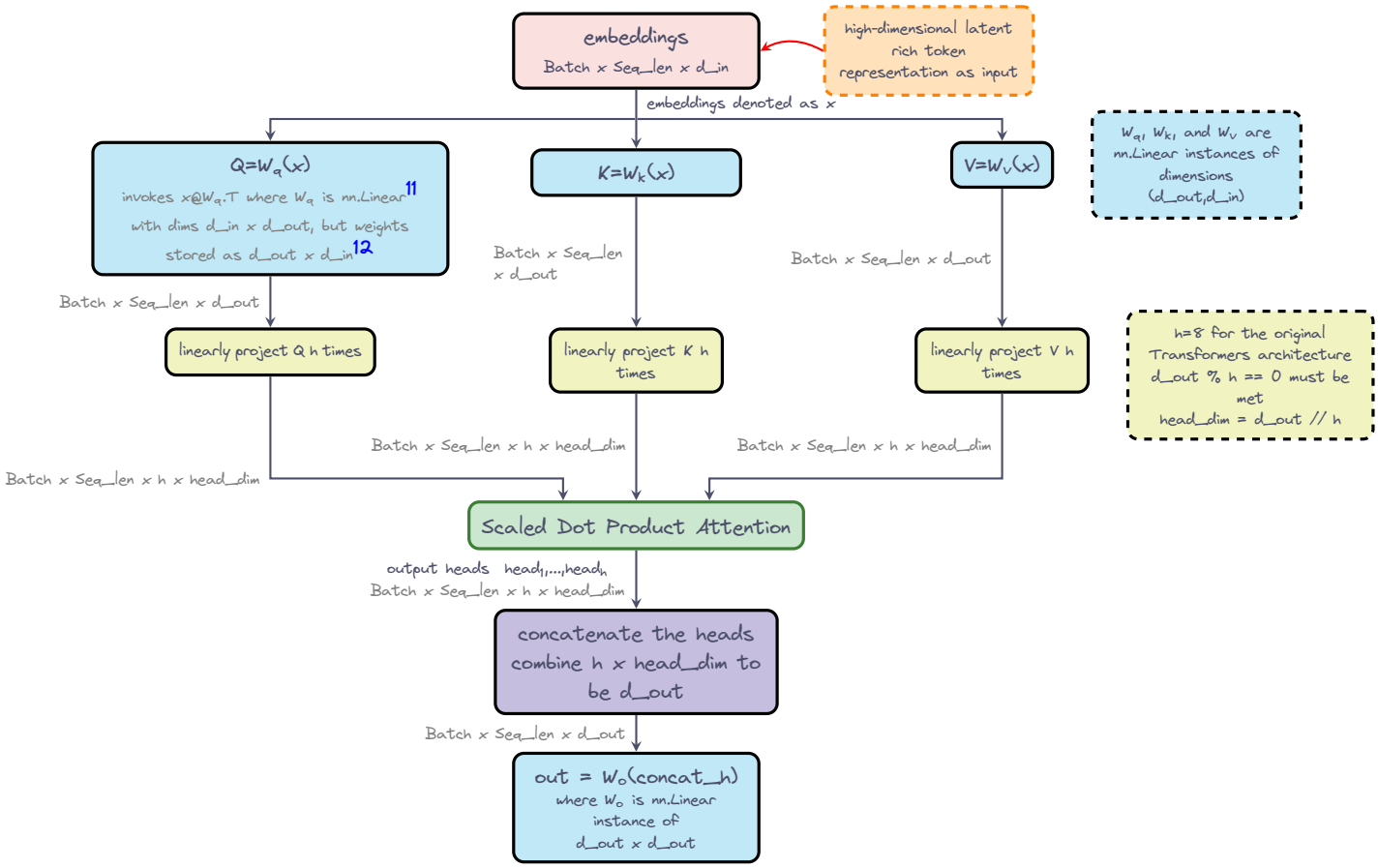
the previously derived mathematical algorithm can then be translated into code as below.

```
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 Attention[13]

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 I 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.

...

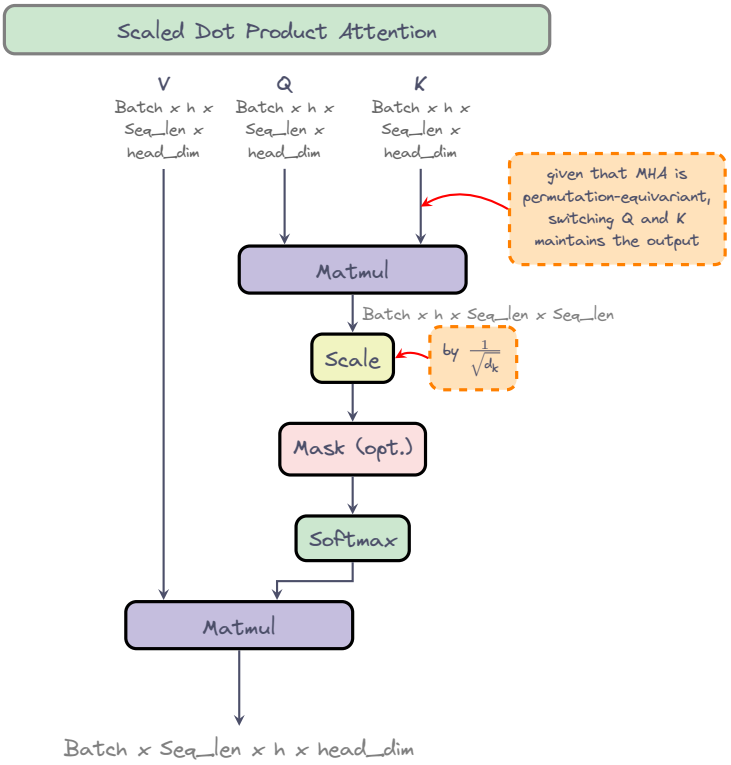
Scaled dot product attention

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 large[14]. 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 previous [13] ...

- ***values*** ~ for each input element, we also have a value vector. This feature vector is the one we want to average over.
- ***score function*** ~ 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 x Seq_len x h x head_dim* before this step where d_k is gotten by *k.shape[-1]*

During the decoding phase, at each step of predicting a word[15], 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 I need the masking block, I 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 tokenizer[16], *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

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

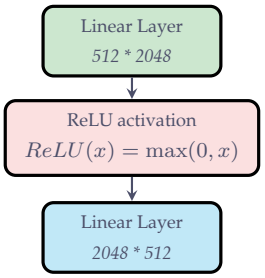
where x is basically the same sequence (as an embedding) input to the $Q, K\&V$. This layer hence is a residual connection necessary for enabling smooth gradient flow through the model and retaining information from the original sequence prior to the multi-head attention. This is simply implemented as

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

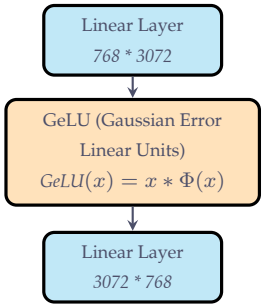
What about the Feed Forward Network layer

Always forming a crucial layer in most models, the FFN, in this case, maps context rich vectors onto a higher dimension[17] which increases learning so it can model more complex relationships and also adds an activation function to introduce non-linear, even better relations.

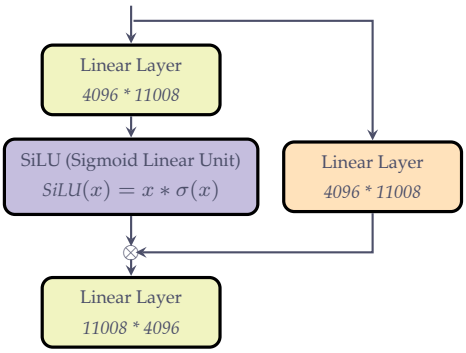
[17] *Feed Forward NN layer for Transformer model*



Feed Forward NN layer for GPT-2



Feed Forward NN layer for Llama-2-7b

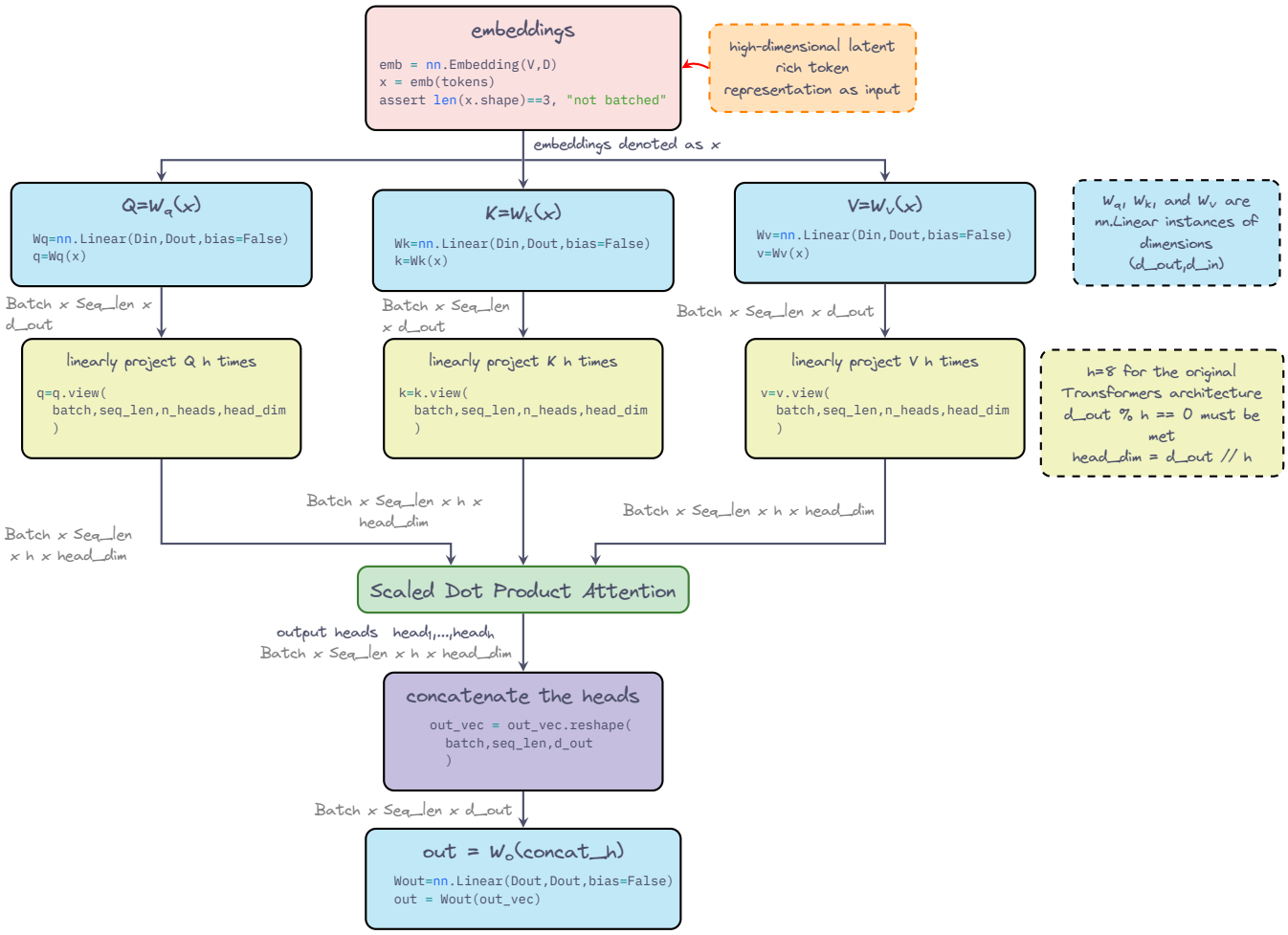


Building Llama-2 from the SDPA outwards...

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



But wait! what about the RoPE implementation, remember that as has been discussed earlier, positional encodings should be somewhere in the above disjointed[18] graph of a code. Let's figure out where?

[18] disjointed for it does not exist in a nn.Module class with the updatable weights in the init part of the class

Recap on Rotational Positional Encoding

```
def precompute_freqs_cis(d, context_len, theta =
    10_000, device = "gpu"):
    #
    #
    assert d % 2 == 0, "dim must be divisible by 2"
    #
    i_s = torch.arange(0,d,2)[:(d//2)].float()
    theta_s = theta ** (- i_s / d).to(device)
    m = torch.arange(context_len, device=device)
    freqs = torch.outer(m, theta_s).float()
    freqs_cis = torch.polar(torch.ones_like(freqs),
        freqs)
    return freqs_cis
```

As the paper[9] says, "…to any $x_i \in R^d$ where d is even…"

$i_s = 2(i-1)$ *for* $i \in \{1, 2, \ldots, d/2\}$

$10000^{-i_s/d}$ *which expands to* $10000^{-2(i-1)/d}$

outer product of $\vec{m}$ *&* $\vec{\theta}$ *to give*

$$\begin{pmatrix} m_1\theta_1, & m_1\theta_2, & \ldots, & m_1\theta_{d/2-1}, & m_1\theta_{d/2} \\ m_2\theta_1, & m_2\theta_2, & \ldots, & m_2\theta_{d/2-1}, & m_2\theta_{d/2} \\ \vdots & \vdots & & \vdots & \vdots \\ m_{cl}\theta_1, & m_{cl-1}\theta_2, & \ldots, & m_{cl-1}\theta_{d/2-1}, & m_{cl-1}\theta_{d/2} \end{pmatrix}$$

elementwise mapping i.e. $m_1\theta_1 \Rightarrow \cos(m_1\theta_1) + i\sin(m_1\theta_1)$ *where the ones are the absolute value arguments*

```
def apply_rotary_embs(x, freqs_cis, device):
    #
    #
    x_c = torch.view_as_complex(
        x.float().reshape(*x.shape[:-1], -1, 2)
    )
    #
    f_c = freqs_cis.unsqueeze(0).unsqueeze(2)
    #
    #
    x_rotated = x_c * f_c
    #
    x_out = torch.view_as_real(x_rotated)
    #
    x_out = x_out.reshape(*x.shape)
    return x_out.type_as(x).to(device)
```

takes each group of 2s of elements,… [x, y], [m, n], … to single elements of x+yj, m+jn…

dynamically expands the last dimension (…,d1) to $\left(\ldots, \frac{d1}{2}, 2\right)$ *where d1 is even*

dims transformed from $(\ldots, d)$ *to* $\left(\ldots, \frac{d}{2}\right)$

reverses the effect of torch.view_as_complex

With the knowledge of the implementation of the rotational positional encodings, let's inject it into the graph for the MultiHead Attention after the transformation

$$[batch \times seq\_len \times n\_heads \times head\_dim]$$

but before the high-dimensional transpose to get the batch of heads each with dimensions (seq_len,head_dim)[19].

[19] reminder that the rotational transformation is to be applied to the queries and keys only and not the values (*refer to page 4*).

$\star$ which is then done below[20]

```
# Already defined earlier
dim=4096; n_heads=32; context_len=4096
Q,K,V=... # each dims being (Batch,SeqLen,Heads,HDim)
m_theta_polar_tensor =
    precompute_freqs_cis(dim//n_heads,
    context_len*2,"cpu")
m_theta_polar_seq = m_theta_polar_tensor[:seq_len]
Q=apply_rotary_emb(Q,m_theta_polar_seq)
K=apply_rotary_emb(K,m_theta_polar_seq)
```

Unwrapping the Transformer Block

As much as the original Transformer does the normalization as

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

Llama2 does a prenormalization given by

$$x_n = \text{RMSNorm}(x)$$

$$\text{out} = x + \text{Multihead}(x_n)$$

where

$$\text{RMSNorm}(x) = \frac{x_i}{\text{RMS}(x)} * \gamma_i$$

$$\text{RMS}(x) = \sqrt{\epsilon + \frac{1}{n}\sum_{i=1}^{n} x_i^2}$$

which works out in code as

```
class RMSNorm(torch.nn.Module):
    def __init__(self, dim: int, eps: float = 1e-5):
        super().__init__()
        self.eps = eps
        self.weight = nn.Parameter(torch.ones(dim))
    def forward(self, x):
        means = x.pow(2).mean(-1, keepdim=True)
        norm_x = x * torch.rsqrt(means + self.eps)
        return (norm_x * self.weight).to(x.dtype)

rmsNorm=RMSNorm(dim) # dim=4096
x_norm=rmsNorm(x) # x => embeddings => (Batch,SeqLen,Dim)
# some mhAttention already instantiated called below
attn_out=mhAttention(x_norm)
# then add
out = x + attn_out
```

with the pre-normalization done to the input to the attention block and to the input to the feed-forward networks.

[20] full neat implementation https://github.com/Marvin-desmond/ScalingViTsAcrossTrainingCompute/blob/main/mha/mha_with_rope.py *Llama 2 Multi-Head Attention with ROPE*

However, the original FFN, as can be seen from the side notes on *pg.9*, does two linear transformations with a ReLU[21] activation function applied between the two linear transformations.

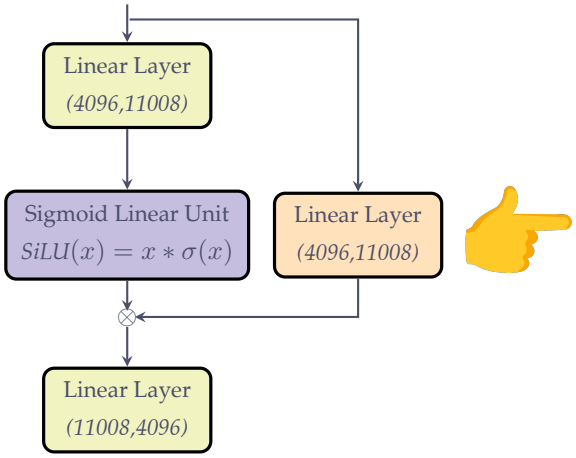
$$FFN(x, W_1, W_2, b_1, b_2) = \max(0, xW_1 + b_1)W_2 + b_2$$

the above equation being representative of the graph computation in the linear topology on the just aforementioned page.
Llama2, the current LLM architecture of interest in implementation in this section of the article, focuses on a Linear Unit known as SwiGLU[22], a variation of the Transformer FFN layer which then uses a variant of the Gated Linear Unit[23]. This leads to the FFN layer having three weight matrices as opposed to the original two which yields the implementation below.

[21] https://proceedings.mlr.press/v15/glorot11a.html
Deep Sparse Rectifier Neural Networks
Glorot et al. 2011

[22] https://arxiv.org/abs/2002.05202v1
GLU Variants Improve Transformer
Noam Shazeer 2020

[23] https://arxiv.org/abs/1606.08415
Gaussian Error Linear Units (GELUs)
Dan Hendrycks, Kevin Gimpel 2016

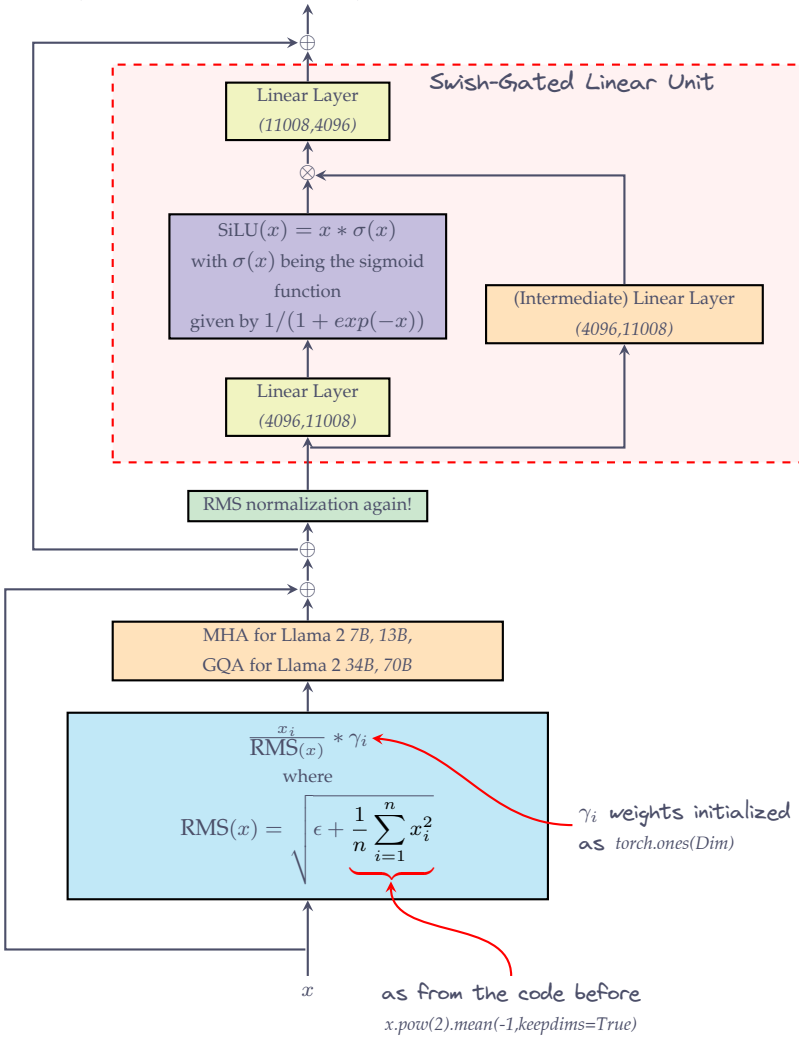



```python
class FeedForward(nn.Module):
  def __init__(self,dim,hidden_dim,bias=False,device="cpu"):
      super(FeedForward,self).__init__()
      self.w1 = nn.Linear(dim,hidden_dim,bias=bias,device=device)
      self.v = nn.Linear(dim,hidden_dim,bias=bias,device=device)
      self.w2 = nn.Linear(hidden_dim,dim,bias=bias,device=device)
      self.SiLU = nn.SiLU()
  def forward(self,x):
      x = (self.SiLU(self.w1(x))*self.v(x))
      x = self.w2(x)
      return x
```

With the $\star$ operation being the Hadamard product, or as commonly known, the elementwise product, of the two Weight matrices of dimensions $(4096, 11008)$ to give a resulting matrix maintaining the given dimensions.
In the general implementation for any given Llama 2 variant, the hidden dimension size is gotten by

- scaling of *dim* by 4
- reduction by $2/3$
- adjust it as a factor of a given multiple for computational efficiency

Hence, from the clarifications, the whole Transformer block is visualized as

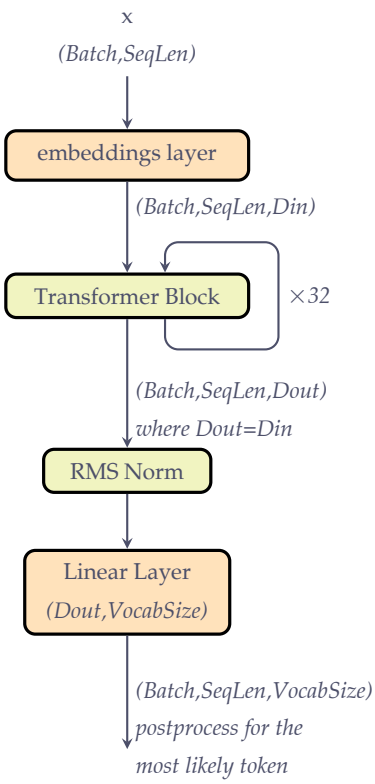


With the above nice input-output mapping translating to code as

```
class TransformerBlock(nn.Module):
    def __init__(self,d_in,d_out,n_heads,context_window,device="cpu"):
        super(TransformerBlock,self).__init__()
        self.rms_attn = RMSNorm(d_in,device=device)
        self.attn = MHAandRoPE(d_in,d_out,n_heads,context_window,device=device)
        self.rms_ffn = RMSNorm(d_in,device=device)
        self.ffn = FeedForward(d_in,4*d_in,device=device)

    def forward(self, x, m_thetas):
        attn_x = self.rms_attn(x)
        h = self.attn(attn_x, m_thetas) + x

        ffn_x = self.rms_ffn(h)
        out_x = self.ffn(ffn_x)
        x = out_x + h
        return x
```

The whole Llama 2 picture

Building this architecture has been interesting, so now let's go out from the Transformer block to the whole Llama 2 model, having a full understanding of the architecture.



for parameters

```
class CONFIG:
    VOCAB: int = 32_000
    CONTEXT_LEN: int = 4096
    DIM: int = 4096
    N_HEADS: int = 32
    N_LAYERS: int = 32
    HIDDEN_DIM: int = 11008
    DTYPE: torch.dtype =
        torch.bfloat16
```

with the model translating to code as

```
class TransformerLlama2(nn.Module):
    def __init__(self, CONFIG: CONFIG, device="cpu"):
        super(TransformerLlama2,self).__init__()
        self.token_embeddings = nn.Embedding(
            CONFIG.VOCAB, CONFIG.DIM,
            device=device)
        self.layers = nn.ModuleList()
        for _ in range(CONFIG.N_LAYERS):
            self.layers.append(
                TransformerBlock(
                    CONFIG.DIM, CONFIG.DIM,
                    CONFIG.N_HEADS, CONFIG.CONTEXT_LEN,
                    device=device))
        self.norm = RMSNorm(CONFIG.DIM, device=device)
        self.output = nn.Linear(
                        CONFIG.DIM,CONFIG.VOCAB,
                        bias=False, device=device
                        )
        self.m_thetas = precompute_freqs_cis(
                CONFIG.DIM//CONFIG.N_HEADS,
                CONFIG.CONTEXT_LEN*2,
                device=device
            )
    def forward(self,x):
        batch, seq_len = x.shape
        x = self.token_embeddings(x)
        m_thetas_seq = self.m_thetas[:seq_len]
        for layer in self.layers:
            x = layer(x, m_thetas_seq)
        x = self.norm(x)
        x = self.output(x).float()
        return x
```

The architecture now complete, the inferencing of the model given the loading of the weights is the key section to follow. However, Large Language Models and in this case Llama2, even though decoder only, is still high memory demanding and so cannot be easily run on local computes. Therefore, inferencing brings into light cloud computes that effectively run inference pipelines.

⋆ The current snapshot for the inference pipeline is now https://github.com/Marvin-desmond/ScalingViTsAcrossTrainingCompute/blob/main/transformerLlama2/local_inference.py

First shot at inference

As much as I would want to look for the cloud instance on AWS with the highest GPU VRAM and spawn it, ssh to it then copy the inference files and folders to the remote instance before running the pipeline, and then worrying about destroying the instance before the expenses gets too high, let's simplify things a bit shall we! As on-demand as I can get and with just focusing on the Python code with a bit of sprinkling of decorators, I'd like to go into this platform called Modal[24]

Configuring Modal

After installing Modal, you can run a python file using

```
modal run hello.py
```

instead of

```
python hello.py
```

To illustrate on the local entry point for Modal in the code, let's say the code in the file is initially

```
def func():
    import subprocess
    try:
        subprocess.run("nvidia-smi")
    except:
        print("CUDA not found")

if __name__ == "__main__":
    func()
```

To have it compatible with cloud running, we'll have to decorate *func* as shown

```
import modal
app = modal.App()

@app.function()
def func():
    import subprocess
    try:
        subprocess.run("nvidia-smi")
    except:
        print("CUDA not found")
```

[24] https://modal.com/docs/examples

the local entry point will now change from

```
if __name__ == "__main__":
    func()
```

to now being

```
@app.local_entrypoint()
def main():
    func.local()
    func.remote()
```

where the function can now be invoked on your local compute using *func.local*() and Modal's remote compute using *func.remote*(), and that's about it! For those familiar with CUDA, it is like prepending the keywords *__host__ __device__* to a function without having to rewrite the whole function for each compute. No need to ssh or maintain any GPU instance! The results for the functions, assuming your local compute is CPU-only, will be

```
CUDA not found
CUDA not found
```

Modal runs on CPU by default for the remote compute, so let's add a GPU option[25], for now going for the T4.

```
import modal
app = modal.App()

@app.function(gpu="T4")
def func():
    import subprocess
    try:
        subprocess.run("nvidia-smi")
    except:
        print("CUDA not found")
```

and for the result!

```
CUDA not found
Wed May 28 20:41:22 2025
+-----------------------------------------------------------------------------------------+
| NVIDIA-SMI 570.86.15              Driver Version: 570.86.15      CUDA Version: 12.8     |
|-----------------------------------------+------------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id          Disp.A | Volatile Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |           Memory-Usage | GPU-Util  Compute M. |
|                                         |                        |               MIG M. |
|=========================================+========================+======================|
|   0  Tesla T4                       On  |   00000000:00:1C.0 Off |                    0 |
| N/A   24C    P8             9W /   70W |       1MiB /  15360MiB |      0%      Default |
|                                         |                        |                  N/A |
+-----------------------------------------+------------------------+----------------------+

+-----------------------------------------------------------------------------------------+
```

25

- T4 ~ 16GB VRAM
- L4 ~ 24GB VRAM
- A10G ~ 24GB VRAM
- A100-40GB
- A100-80GB
- L40S ~ 48GB VRAM
- H100 ~ 80GB VRAM
- H200 ~ 141GB VRAM
- B200 ~ 180GB VRAM

Configuring the pipeline for GPU inference

Now that I have a good enough understanding of Modal, let's configure the file *local_inference.py* for remote compute.

We'll need torch for GPU accelerated numerical computing, huggingface hub for downloading llama weights, sentencepiece as the tokenizer package for Llama2. So let's create an image that has those packages, and also upload the corresponding necessary files to remote that defines the classes and utilities for the model implementation.

```
import modal
app = modal.App("llama-gpu-inference")
image = modal.Image.debian_slim().pip_install(
    "torch", "numpy", "sentencepiece",
    "huggingface_hub[hf_transfer]"
    ).env({"HF_HUB_ENABLE_HF_TRANSFER": "1"}
    ).add_local_file(
        local_path="./core.py",remote_path="/root/core.py"
    ).add_local_file(
        local_path="./block_utils.py",remote_path="/root/block_utils.py"
    ).add_local_file(
        local_path="../pos_freqs.py",remote_path="/root/pos_freqs.py"
    ).add_local_dir(local_path="../mha", remote_path="/root/mha")
```

Let's then provision a Modal volume for saving the weights.

```
from pathlib import Path
volume = modal.Volume.from_name("model-weights-vol",
    create_if_missing=True)
MODEL_DIR = Path("/models") # note the dot is removed
```

Next, I make the function to download model weights run on remote compute by decorating it as follows

```
@app.function(
  volumes={MODEL_DIR: volume},
  image=image,
  secrets=[modal.Secret.from_name("huggingface-secret")])
def download_model(
    repo_id: str="meta-llama/Llama-2-7b",
    revision: str=None,  # include a revision to prevent
        surprises!
    ):
    # more code below ...
```

and by changing the function call as[26]

```
download_model.remote()
```

[26] ensure the huggingface secret is configured since Llama weights access requires authentication, and also remove the

```
from dotenv import load_dotenv
load_dotenv()
```

and

```
if not torch.cuda.is_available():
    sys.exit(0)
```

snippets of codes from the original *local_inference.py* code file for it to work with the remote compute.

Choosing the right GPU

This is the core question for us to choose the GPU that fits our memory needs during inference whilst also being economical but not by reducing the reliable output of tokens/sec. We cannot use the T4 because as this equation states[27], the gpu memory (in GB) denoted as M is given by

$$M = \left(\frac{P \times 4B}{32/Q} \right) \times 1.2$$

where

$P \sim$ amount of parameters in the model

$4B \sim$ 4 bytes, the bytes used for each parameter

$32 \sim$ there are 32 bits in 4 bytes

$Q \sim$ amount of bits for loading the model, 16 bits, 8 bits, or 4 bits

$1.2 \sim 20\%$ overhead of additional loading in GPU memory

For *Llama2 model 7B*, which obviously has 7B[28] parameters, currently being inferenced at full precision, hence yielding Q as 32, the lower bound for GPU is then

$$M = \left(\frac{7 \times 10^9 \times 4}{32/32} \right) \times 1.2$$

$$M = 3.36 \times 10^{10} \text{ bytes}$$

$$M = 33.6\, GB$$

Hence for the GPU options by Modal, I can then go for the nearest upper GPU which is A100-40GB. This leads to decorating the class below as

```
@app.cls(
        gpu="A100-40GB",
        volumes={MODEL_DIR: volume},
        image=image
        )
class PIPELINE:
    # more code ...
    device = "cuda"
```

and interesting changes to the *__init__* and the *inference* methods[29].

[27] Calculating GPU memory for serving LLMs

[28] what if I didn't know the number of parameters? Well for starters, I can get the parameters of filters in convolution layers by knowing the number of filters and the number of channels per each input to that layer and the kernel size (depthwise stack of kernels form a filter). For a Linear layer, I get the size of the weight matrix and the bias to compute the parameters in that layer.

[29]

```
    def __init__(self, device):
        # ...
```

becomes

```
    @modal.enter()
    def enter(self):
        # ...
```

and the inference method is decorated as

```
    @modal.method()
    def inference(self):
        # ...
```

with the function call being changed to

```
@app.local_entrypoint()
def main():
    download_model.remote()
    pipeline = PIPELINE()
    pipeline.inference.remote()
```

And so trying this prompt

The interesting life of the blue eyed child from a glass orb

gives

The interesting life of the blue eyed child from a glass orb. A story of the unusual life of a young girl who grew up in the midst of the great depression. She saw a lot in her short life. It's a heart warming story of a little girl who grew into a wonderful woman. This is a biography of a woman who grew up in the south during the Great Depression, who then worked her way through college and became a successful attorney and judge. It's the story of a young girl who grows up in the midst of the depression and becomes a successful attorney. It's a great story with a lot of heart. I loved this book. It was such a great read. I loved the story of a girl growing up in the midst of the depression, and how she made her way through life. This is a wonderful story about a young girl who grew up in the midst of the Great Depression and how she was able to make it through. She was a strong and determined young woman and her story is very inspiring. I would recommend this book to anyone. This is a very interesting and inspiring story. It is the story of a young girl growing up in the midst of the Great Depression and how she was able to make it through. She was a strong and determined young woman and her story is very inspiring...

From Transformers To Vision Transformers

Revealing The Motivation

The YouTube recommendation, being as tuned as ever to the videos I liked to watch, recommended me this one video[30]. And of course, developers from DeepMind being the first to present was an awesome start to the video, having loved the kind of impactful research DeepMind does, AlphaFold 2[31] being the first of many that stuck in my mind.

This video goes into optimization using Jax[32], as I would call it, a framework that's so powerful at granular and complex differentiation and JiT compiles to GPU and TPUs, a very interesting combo for High Performance Computing. Imagine wanting to build ML workloads in an efficient of code as you can possibly get.

A study done, presented by one Kathleen, gives a walkthrough on the speed and cost of training a ViT[33] given different performance metrics quantifying how fast training gets.[34] This precursor study was a huge stepping stone to training Gemma group of models by Google, *Gemma 3n*[35] being my most beloved, given it was focused on optimization and hence inference for relatively lower memory-constrainted devices.

The focus of the article

With this in mind, the article will now convert the previous Llama 2 architecture to the base Transformer model for which the Google *ViT* is based upon, before now looking into the ViT paper on changes to achieve the final Vision Transformers state. However, I am still in the single-GPU pipeline, hence changes need be made to the architecture to shard it across many GPUs, optimizing it even by float point precision levels as I tune it to its optimal state ever.

So why Vision Transformers?

Given the interesting nature of Transformers of being computationally efficient and scalable, allowing training models of unprecedented size with no sign of saturating performance, and convolutional architectures being so good at computer vision, the research on *ViTs* aimed at improving Transformer models for image capabilities.

[30] https://www.youtube.com/watch?v=vKcA094FSMk
Demo: Gemma 2 architecture: JAX, Flax, and more

[31] https://deepmind.google/discover/blog/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology/
AlphaFold: a solution to a 50-year-old grand challenge in biology

[32] https://cloud.google.com/blog/products/ai-machine-learning/guide-to-jax-for-pytorch-developers
The PyTorch developer's guide to JAX fundamentals

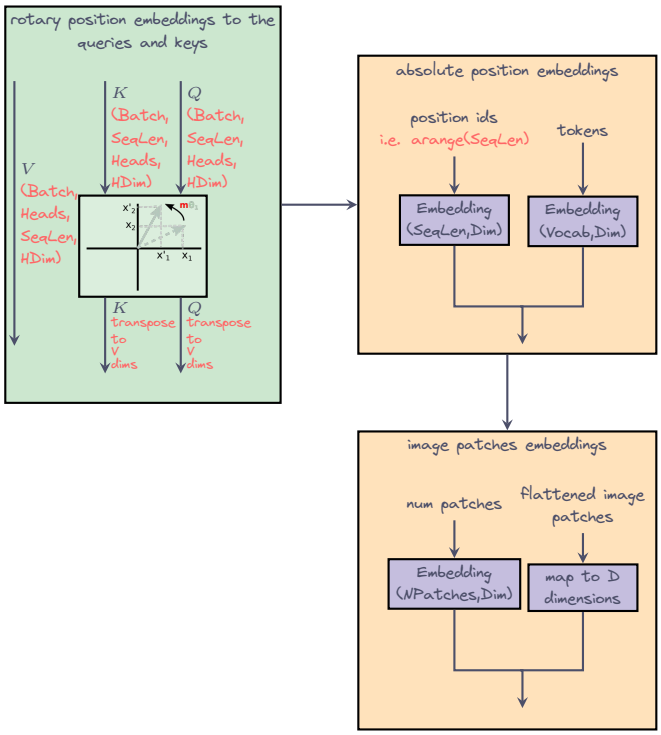
[33] arXiv:2010.11929
An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale
Dosovitskiy et al. 2020

[34] ViT PyTorch vs JAX training benchmarks on Vertex AI Training Platform

[35] https://www.youtube.com/watch?v=eJFJRyXEHZ0
Announcing Gemma 3n Preview: Powerful, Efficient, Mobile-First AI

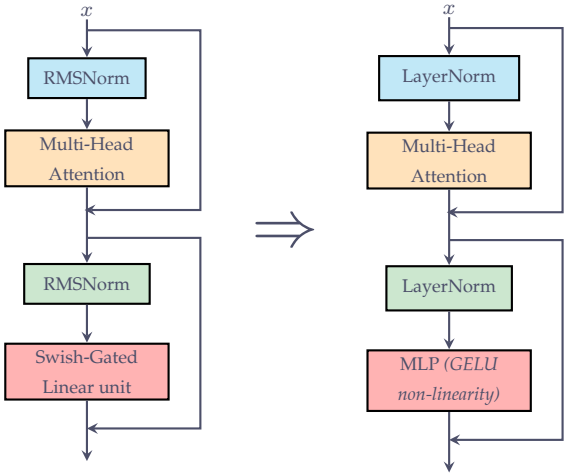
Dumbing down Llama2 to base ViT

First looking at the inner most part of Llama2, the Scaled Dot Product Attention, the rotary positional embedding to the queries and keys is removed and instead the GPT-2 absolute positional embeddings used, however in this case the image patches are considered instead of tokens.



Moreover, *ViT* has no masking of the intermediate attention scores hence its attention mechanism is non-causal.

Within the Transformer Block, normalization changes from *RMSNorm* to *LayerNorm*, computed for the inputs before the attention and the feedforward blocks.



Understanding the image embeddings for ViT

Going onto the interesting part of what makes this pioneering research awesome, is how the image patches is handled. As described in *page 3 section 3.1* of the paper[33], *we reshape the image* $x \in R^{H \times W \times C}$ *into a sequence of flattened 2D patches* $x_p \in R^{N \times (P^2 \cdot C)}$, *where* (H, W) *is the resolution of the original image,* C *is the number of channels,* (P, P) *is the resolution of each image patch, and* $N = HW/P^2$ *is the resulting number of patches, which also serves as the effective input sequence length for the Transformer.*

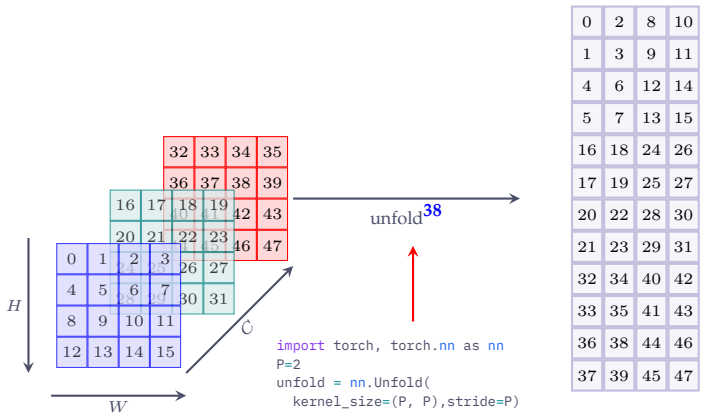
Let's implement this process in two ways

- using torch unfold
- using einops Rearrange

torch unfold

PyTorch is an awesome framework, and with it comes one nice functionality, *torch unfold*[36], the functionality behind the very core convolution operations in convolutional neural networks. So how does it work?

Imagine I have a 3-channel tensor, then *unfold* extracts the patch of a given kernel size across all channels in the tensor and unrolls it to a single column, before proceeding to the next patch as noted by the stride[37].



0	2	8	10
1	3	9	11
4	6	12	14
5	7	13	15
16	18	24	26
17	19	25	27
20	22	28	30
21	23	29	31
32	34	40	42
33	35	41	43
36	38	44	46
37	39	45	47

Next, let's create patches from an image and visualize them for the different kernel sizes. Let's consider this image I once used in the *From Tensors to Residual Learning*[39] course which I taught in PyTorch and focused on the fundamentals of Deep Learning from the mathematics of Calculus to implementing the different variants of residual network architectures.

[36] Unfold
PyTorch API reference

[37] the tensor needs extrusion to the batch dimension since unfold only supports 4-D tensors

[38] Note that *unfold* gives us the flattened 2D patches as a transpose of the expected 2D patches in the paper, since I have in the resulting visual $(P^2 \cdot C) \times N$ when I need its transpose, denoted as x_p in the paper of dims $N \times (P^2 \cdot C)$. This will be handy later on!

[39] *From Tensors To Residual Learning*
From the math of tensors to the implementation of residual learning

Huggingface datasets 🤗 come in handy for this, getting the image which is a *Pillow* instance which I then transform to a *torch Tensor*

```
from datasets import load_dataset
from  torchvision.transforms.v2.functional import (
    pil_to_tensor, resize)
# function to resize the image to 240 by 240
resize_fn = lambda x, size=240: resize(
    x, size=[size,size]).to(torch.float32)

dataset = load_dataset("huggingface/cats-image")
image = dataset['test']['image'][0]
image = pil_to_tensor(image)
image = resize_fn(image)
C,H,W=image.shape
```

Let's of course initialize the unfold instance. We want to get, for now, 4 patches from the image, this means the patch size is

$$N = HW/P^2 \Rightarrow 4 = (240/P)^2 \Rightarrow P = 120$$

```
P=120
unfold = nn.Unfold(kernel_size=(P, P),stride=P)
patches = unfold(image)
print(patches.shape) # torch.Size([1, 43200, 4])
```

and so the patches can be converted to images as

```
def extractPatch(patches, index, P):
    patch = patches[...,index].view(1,3,P,P)
    patch = patch.squeeze(0).permute(1,2,0)
    return patch.to(torch.uint8).numpy()
```

and visualize[40] the image patches using the code

```
showPatches(patches,N,P)
```

to get

40

```
import matplotlib.pyplot as plt

def showPatches(patches, N, P):
    rows=cols=int(N**.5)
    for i in range(N):
        plt.subplot(rows,cols,i+1)
        patch_image = extractPatch(patches, i, P)
        plt.imshow(
            patch_image,aspect = "auto"
            )
        plt.tight_layout()
        plt.xticks([]); plt.yticks([])
    plt.subplots_adjust(
    hspace=0.1,wspace=0.1 # wspace => aspect auto
    )
    plt.show()
```

The next big thing, einops[41]

This library greatly simplifies a lot of incredible operations, and is greatly used even in simplifying high dimensional matrix-multiplication heavy layers in many model graphs. The docs is wonderful and on the side notes for in-depth review. In this case, I want to get the image dimensions, and then get the height and width as integer multiples of the patch size, but I need to be cautious on how I handle the channel dimensions, that is, how I translate the unfold operation as either channel dimensions first or spatial dimensions first. This change in dimensions is implemented using einops as

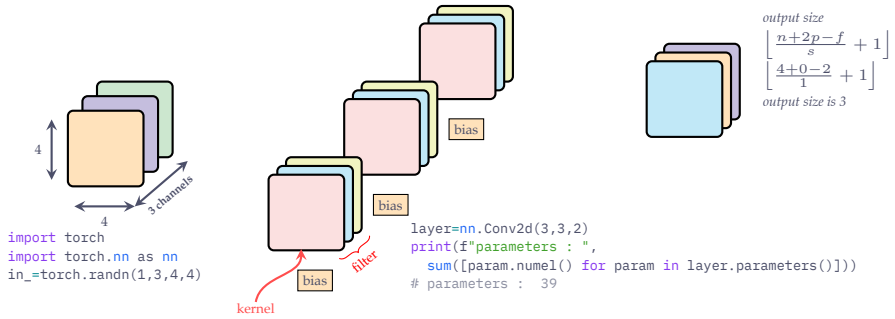
```
from einops.layers.torch import Rearrange
rearr = Rearrange(
    'b c (h p1) (w p2) -> b (c p1 p2) (h w)',
    p1 = P, p2 = P)
```

considering that the image is already a 4D tensor. The above operations says, hey, let's take subsets of the spatial dimensions across all channels, then rearrange the dimensions to a batch of these tensors of size $P^2 \cdot C$, N of such, dimensions denoted as $(1, P^2 \cdot C, N)$. Reminder that this is the transpose of x_p. It can be invoked to get the image patches which then gives the same results as the visual just above.[42]

```
patches_again = rearr(image)
showPatches(patches_again,N,P)
```

torch convolution

I've always loved convolution, because I love signal processing, and I love image processing, and I love Computer Vision. This operation is core in many topics across these domains. Convolution neural networks is inspired by the biological cortex and I've gone through it in-depth in my course[43].



[41] https://einops.rocks/pytorch-examples.html
Writing a better code with pytorch and einops

[42] Note that as I understood from [38], I have to transpose how I actually got the patches to

```
Rearrange('b c (h p1) (w p2) -> b (h w) (p1 p2 c)',
        p1=P,p2=P)
```

which then gives us the 2D flattened patches $x_p \in R^{N \times (P^2 \cdot C)}$.

[43] https://youcanjustbuild.com/courses/from-tensors-to-residual-learning/foundations
The foundations of residual learning

Now onto implementing the image embeddings

Using convolution, I implicitly get the image patches and linearly project to D dimensions directly. The kernel size becomes the size of the needed patch with the stride being the same, the output channels size become D[44]. This layer is also essential given it is a trainable layer, as opposed to the two previously looked-into ops that weren't.

```
patch_layer=nn.Conv2d(3, 768, kernel_size=16, stride=16)
```

Based on the output size from the convolution formula, I get

$$\left\lfloor \frac{256 - 16}{16} + 1 \right\rfloor = 16$$

which begets the output size of 16×16 with 768 channels in the order $(1, 768, 16, 16)$. Looking into this output, it aligns more with $(1, D, \sqrt{N}, \sqrt{N})$ when what I need is $(1, N, D)$. Hence, I consider two operations, combining the last two dimensions then transposing the now new last two dimensions, programmatically implemented as

```
in_ = torch.randn(1,3,256,256)
out = patch_layer(in_)
out = out.flatten(2) # flatten from dim 2, zero-indexed
patch_embs = out.transpose(1,2)
```

The output of this projection is known as the *patch embeddings*. We then need to prepend a class token[45] to the sequence of embedded patches

$$[\mathrm{x}_{\text{class}}; \mathrm{x}_p^1\mathbf{E}; \mathrm{x}_p^2\mathbf{E}; \cdots; \mathrm{x}_p^N\mathbf{E}]$$

```
cls_token = nn.Parameter(torch.randn(1, 1, dim))
x = torch.cat((cls_token,patch_embs),dim=1)
```

Adding positional embeddings to the patch embeddings

By simplifying their learning embedding from the advanced 2D-aware position embedding due to no significant performance, the paper uses 1D position embeddings defined by $E_{pos} \in R^{(N+1)\times D}$.

```
position_embeddings = nn.Parameter(
    torch.randn(1,N+1,dim))
```

which is then added to the augmented patch embeddings

[44] the original ViT uses image resized to 256 with patch size of 16 and D being 768 for *ViT-Base 16*. *patch_dim* is basically $C \times P^2$.

[45] In the interesting implementing of *Vision Transformers*, some *10x* engineers opted for toggling between mean pooling and cls tokens computed with the original patch embeddings. You can see their awesome implementation of such in their codebase https://github.com/lucidrains/vit-pytorch/blob/main/vit_pytorch/vit.py

```
x += pos_embeddings[:,(N+1)]
```

and that is it to give us the whole implementation as

```
class ImageEmbeddings(nn.Module):
    def __init__(self, H, W, P, dim):
        super(ImageEmbeddings,self).__init__()
        N = int((H*W)/(P**2)); self.N = N
        assert H%P==0 and W%P==0, \
          "image size must be integer multiple of patch"
        self.conv_then_project = nn.Conv2d(
            3,out_channels=dim,kernel_size=P,stride=P)
        self.cls_toks = nn.Parameter(torch.randn(1, 1,
            dim))
        self.pos_embeds =
            nn.Parameter(torch.randn(1,N+1,dim))
    def forward(self,image):
        x = self.conv_then_project(image)
        x = x.flatten(2); x = x.transpose(1,2)
        cls_toks = self.cls_toks.expand(x.shape[0],-1,-1)
        x = torch.cat((cls_toks,x),dim=1)
        x += self.pos_embeds[:,:(self.N+1)]
        return x
```

The Looping transformer Block

From the embeddings layer, ViT implements a loop of alternating MultiHeadAttention and MLP blocks, shown previously in the *RMSNorm* to *LayerNorm* section, with LayerNorm applied before every block, and residual connection after every block[46]. As also discussed, the MultiHeadAttention is not masked since it is bidirectional. The Hence, the resulting implementation for the MultiHeadAttention removes RoPe mechanism and masking to be

```
class MultiHeadAttention(nn.Module):
    def __init__(self,d_in,d_out,n_heads,bias=True):
        super(MultiHeadAttention,self).__init__()
        assert d_out%n_heads==0, "d_out must be integer
            multiple of n_heads"
        self.head_dim = int(d_out / n_heads)
        self.n_heads = n_heads
        self.Wq = nn.Linear(d_in,d_out,bias=bias)
        self.Wk = nn.Linear(d_in,d_out,bias=bias)
        self.Wv = nn.Linear(d_in,d_out,bias=bias)
        self.Wo = nn.Linear(d_out,d_out,bias=bias)
```

[46] ViT-Base has the two blocks, MultiHeadAttention and MLP, looped 12 times, meaning 12 layers of the Transformer Block. ViT-Base encompasses ViT-B/16 and ViT-B/32, with the values after the slash being for the patch sizes.

```
    # ...
    def forward(self,x):
        B,seq_len,d_in = x.shape
        q = self.Wq(x); k = self.Wk(x); v = self.Wv(x)
        q = q.view(B,seq_len,self.n_heads,self.head_dim)
        k = k.view(B,seq_len,self.n_heads,self.head_dim)
        v = v.view(B,seq_len,self.n_heads,self.head_dim)
        q = q.transpose(1,2)
        k = k.transpose(1,2)
        v = v.transpose(1,2)
        scores = q @ k.transpose(-1,-2)
        scores = scores / k.shape[-1]**.5
        norm_scores =
            nn.functional.softmax(scores,dim=-1)
        y = norm_scores @ v
        out = y.transpose(1,2).contiguous().view(
               B,seq_len,d_in)
        out = self.Wo(out)
        return out
```

The next block after the residual connection proceeding the MHA is two linear transformations separated by a GELU activation.

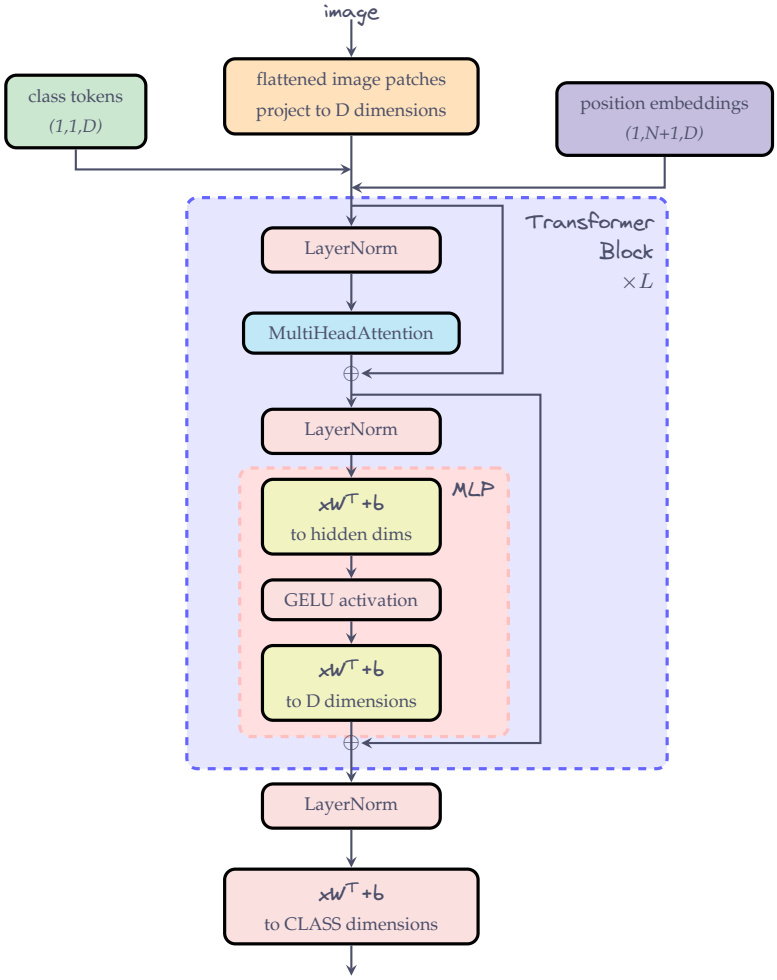
```
class MLP(nn.Module):
    def __init__(self,dim,hidden_dim,bias=True):
        super(MLP,self).__init__()
        self.fc1 = nn.Linear(dim,hidden_dim,bias=bias)
        self.fc2 = nn.Linear(hidden_dim,dim,bias=bias)
        self.act = nn.GELU(approximate='tanh')
    def forward(self,x):
        x = self.fc1(x)
        x = self.fc2(self.act(x))
        return x
```

And hence the complete Transformer Block with LayerNorm before and residual connection after the *MHA* and the *MLP*[47] is beautifully implemented as a PyTorch module as follows

```
class ViTBlock(nn.Module):
    def __init__(self,CONFIG):
        super(ViTBlock,self).__init__()
        self.ln1 = nn.LayerNorm(CONFIG.D_IN)
        self.attn =
            MultiHeadAttention(CONFIG.D_IN,CONFIG.D_OUT,CONFIG.HEADS)
        self.ln2 = nn.LayerNorm(CONFIG.D_IN)
        self.mlp = MLP(CONFIG.D_IN,CONFIG.HIDDEN_DIM)
    def forward(self,x):
        x = x + self.attn(self.ln1(x))
        x = x + self.mlp(self.ln2(x))
        return x
```

[47] as shown in the figure at the end of page 21

And with that, the whole model stands out as




```
class VisionTransformer(nn.Module):
    def __init__(self,CONFIG):
        super(VisionTransformer,self).__init__()
        self.image_embeddings = ImageEmbeddings(
            CONFIG.H, CONFIG.W,
            CONFIG.P,CONFIG.D_IN
        )
        self.vit_blocks = nn.Sequential(
            *[ViTBlock(CONFIG)
              for _ in range(CONFIG.LAYERS)])
        self.norm = nn.LayerNorm(CONFIG.D_IN)
        self.out_linear =
            nn.Linear(CONFIG.D_IN,CONFIG.CLASSES)
    def forward(self,x):
        x = self.image_embeddings(x)
        x = self.vit_blocks(x)
        x = self.norm(x[:, 0])
        x = self.out_linear(x)
        return x
```

Inferencing using ViT-B/16

The specific model *ViT-B/16* is named so because it uses a patch size of 16 and is the base variant of ViT from those implemented in the paper, all base variants having features

Layers	Hidden size D	MLP size	Heads	Params
12	768	3072	12	86M

Taking a model roughly pretrained on the cifar10 dataset, let's copy the weights to the model and do some rough inferencing before I then explore the following variants that we'll now optimize, *ViT-L16,ViT-H14, ViT-g14, ViT-G14*, with the last two variants presented in the paper [48]that looks into the scaling properties as a key to designing future generations effectively. The inference pipeline is interestingly implemented and then can be invoked as [49]

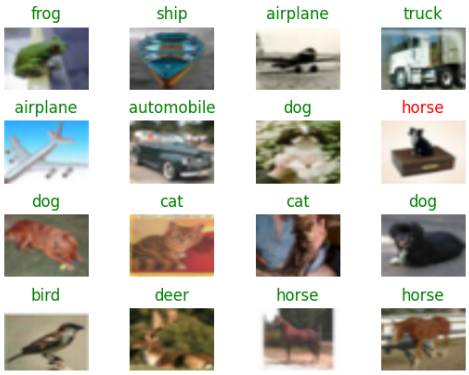
```
vit = VisionTransformer(CONFIG)
weights = torch.load(
    "../models/vit_b_16_pretrained_cifar10.pth",
    weights_only=True, map_location='cpu')
copy_model_weights(vit, weights)
vit = vit.to(device); vit.eval()

classes = ['airplane','automobile','bird','cat','deer',
    'dog','frog','horse','ship','truck']
inv_transforms = Compose([
    Normalize(mean = [-i/j for i,j in zip(MEAN,STD)],
              std = [1/i for i in STD]),
    Lambda(lambda x: x * 255),
    Lambda(lambda x: x.permute(1,2,0)),
    Lambda(lambda x: x.to(torch.uint8))
])

iter_loader = iter(test_loader)
images, labels = next(iter_loader)
images = images.to(device)
with torch.no_grad():
    preds = vit(images)

for i, (image, label) in enumerate(zip(images,labels)):
    plt.subplot(4,4,i+1)
    pred = preds[i,:].argmax(dim=-1).item()
    cls = classes[pred]
    image = image.cpu().squeeze()
    inv_image = inv_transforms(image)
    plt.imshow(inv_image,aspect='auto')
    plt.axis('off')
    plt.title(f'{cls}',color='g' if pred == label else 'r')
plt.subplots_adjust(hspace=0.5,wspace=0.5)
plt.show()
```

[48] arXiv:2106.04560
Scaling Vision Transformers
Zhai et al. 2022 (The infamous Lucas Beyer is also a co-author on this)

[49] the core_utils.py in the directory https://github.com/Marvin-desmond/ScalingViTsAcrossTrainingCompute/blob/main/transformerViT implements the weight copying function and the rest of the inference code can be found in the *core.py* file with the configs for *ViT-B/16* being

```
class CONFIG:
    P = 16
    H = 224
    W = 224
    D_IN = 768
    D_OUT = D_IN
    HEADS = 12
    LAYERS = 12
    HIDDEN_DIM = D_IN * 4
    CLASSES = 10
```

the result of the inference gives



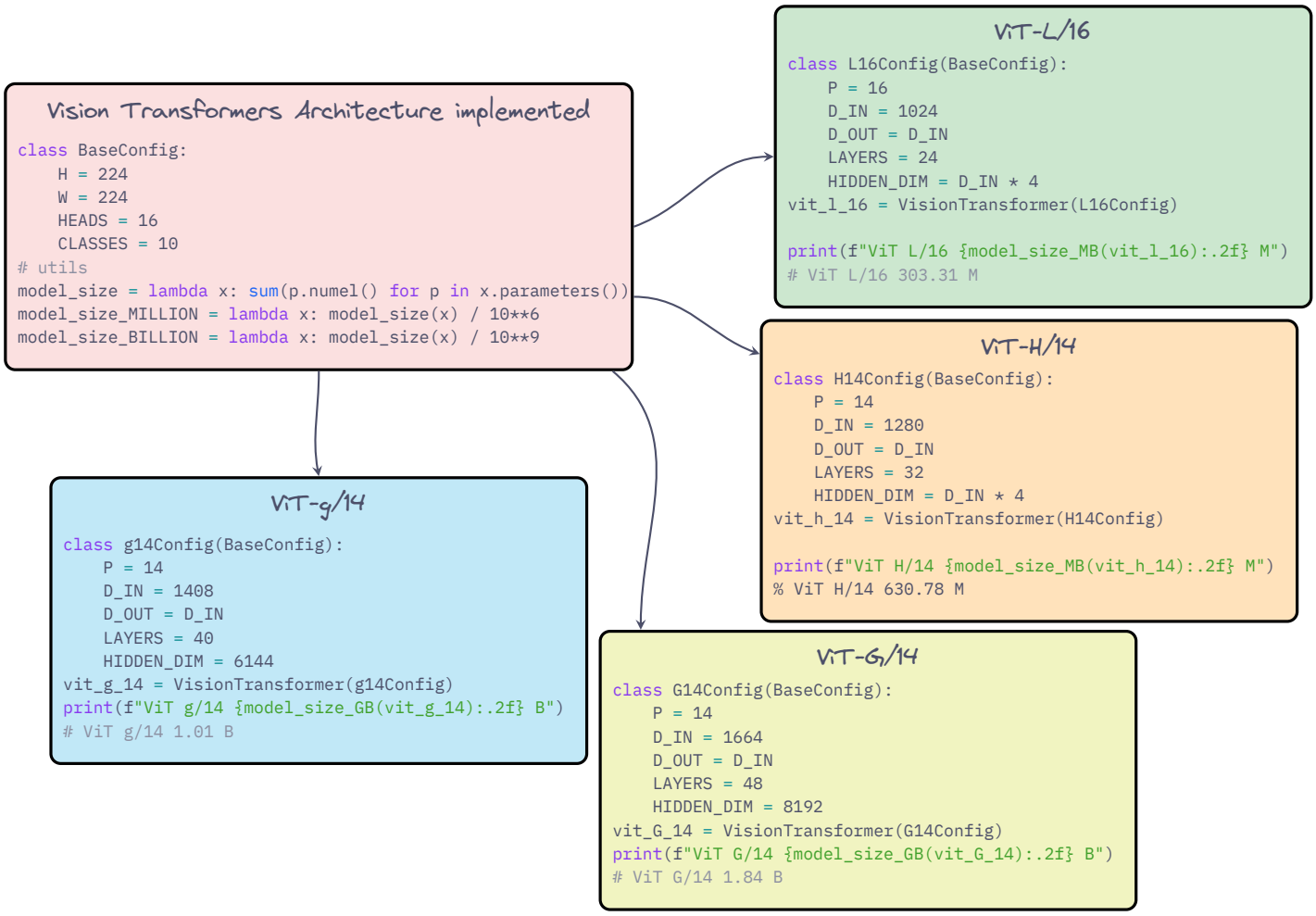
The Four Variants of the "Optimization Apocalypse"

Revisiting the original *Vision Transformers* paper, I see that *ViT-L16* can be grouped as a large variant with patch size 16, and *ViT-H14* can be put in the huge variant with patch size 14. Image size is 224 pixels for the experiments done in the paper hence we'll hold on that for the rest of the article section.

The variants *ViT-g14* and *ViT-G14* are from the next paper [48] and are scaled versions of the earlier models trained to benchmark performance during scaling under different conditions. The summary for the models are then thus (*as extracted from Table 1 and 2 of the respective papers*)

Type/Patch	Depth (Layers)	Dimensions D	Intermediate MLP Size	Heads	Params
L/16	24	1024	4096	16	307M
H/14	32	1280	5120	16	632M
g/14	40	1408	6144	16	1.011B
G/14	48	1664	8192	16	1.843B

which then translates programmatically to



The naive data pipeline

The benchmarking of the *ViT* variants by Google DeepMind from the naive pipeline then scales it to data parallel pipeline using PyTorch's *Distributed Data Parallel* for models that fit into a single gpu,(*refer to the github doc*[34]). We may not explore huge models that need be fit in many gpus given the article is already too long enough, but this will be interestingly explored sooner in a later article that will also go into the interesting *DiLoCo*[50] which is used to revolutionalize multi-node training in a high fault networked training[51]. For the *ViT-G14*, the Fully Sharded Data Parallel (FSDP) is used instead.

Let's now start on building the naive pipeline and use the time in hours per epoch for how much speed improvement I get during optimization even in the model graph using *torch.compile* and float precision reduction in the computations.

Everything starts with cifar10[52]*dataset*

This dataset is infamous for scaling of models, and awesome papers such as one by Keller Jordan[53], shows how much still can be explored based on it. It can be loaded from the torchvision datasets

```
import torch, torchvision
from torchvision.transforms.v2 import (
    Compose, ToImage, Resize, ToDtype, Normalize)
SEED = 42; torch.manual_seed(SEED)
MEAN = [0.485,0.456,0.406]; STD = [0.229,0.224,0.225]
transforms = Compose([
  Resize((224, 224)),ToImage(),
  ToDtype(torch.float32,scale=True),Normalize(MEAN,STD),
])

train_data = torchvision.datasets.CIFAR10(
    root="../datasets", train=True, transform=transforms,
         download=True)
test_data = torchvision.datasets.CIFAR10(
    root="../datasets", train=False, transform=transforms,
         download=True)

print(f"Train images: ", len(train_data)) # Train images:  50000
print(f"Test images: ", len(test_data)) # Test images:  10000
```

The batch will be scaled as per the training limits as from the table in the github optimization docs, but for now, let's consider *Yann Lecun*'s

> *Friends don't let friends use mini-batches larger than 32*

[50] arXiv:2311.08105
DiLoCo: Distributed Low-Communication Training of Language Models
Douillard et al. 2023

[51] Fault Tolerant Llama: training with 2000 synthetic failures every 15 seconds and no checkpoints on Crusoe L40S
Tristan Rice, Howard Huang
June 20, 2025

[52] https://www.cs.toronto.edu/~kriz/cifar.html
The CIFAR-10 dataset
Thanks Hinton and the team

[53] arXiv:2404.00498
94% on CIFAR-10 in 3.29 Seconds on a Single GPU
Keller Jordan

Now that I know the batch size to use, let's implement the iterable for batched data processing

```
from torch.utils.data import DataLoader
BATCH=32
train_loader = DataLoader(train_data,batch_size=BATCH,shuffle=True)
test_loader = DataLoader(test_data,batch_size=BATCH,shuffle=True)
```

And then now, let's start with the model benchmark for ViT-L/16. Instantiating it becomes easy, considering we've gone through it clearly.

```
vit_l_16 = VisionTransformer(L16Config)
device = (torch.accelerator.current_accelerator().type
          if torch.accelerator.is_available() else "cpu")
vit_l_16 = vit_l_16.to(device)
vit_l_16.train()
```

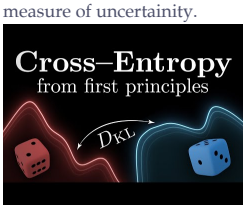
Next, let's define the optimizer that updates the weights with respect to the gradients computed and the cross entropy[54] loss function, the one for which invoking backward propagation computes the needed gradients. I explain a lot more about gradient computation and backpropagation in this course [55]and specifically the section for which the link directs.

```
optimizer = torch.optim.SGD(
    vit_l_16.parameters(),lr=1e-3,momentum=.9)
criterion = torch.nn.CrossEntropyLoss()
```

onto training for a single epoch and computing the time per epoch hours, then

```
    import time
    from tqdm import tqdm
    start = time.time()
    running_loss = 0.0
    for i, (images, labels) in enumerate(tqdm(train_loader)):
        images = images.to(device)
        actual = labels.to(device)
        optimizer.zero_grad()
        predicted = vit_l_16(images)
        loss = criterion(predicted,actual)
        running_loss += loss.item()
        if i % 200 == 0:
          last_loss = running_loss / 200
          print(' BATCH {} LOSS: {:.2f}'.format(i + 1, last_loss))
          running_loss = 0.
        loss.backward()
        optimizer.step()
    stop = time.time()
    print(f"time : {(stop - start) / 3600:.5f} hours per epoch")
```

[54] This video awesomely delves into probability and cross-entropy. Its baseline concept is entropy, which is a measure of uncertainity.



The Key Equation Behind Probability
by Artem Kirsanov

[55] *From Tensors to Residual Learning*
Playing with Grads

Time in Hours per Epoch: Part One

The metric of priority is time in hours per epoch. Considering batch size of 32 for a start, trying to run this on the *T4* free GPU tier of 16GB VRAM in Google Colab crashes since training requires more memory than the available VRAM, so, the options to not run out of memory involve:

- reduce the batch size, training will run but with no speed improvement, and I need to reduce it.
- mixed-precision training, trains some layers, i.e. convolution layers on float16 which makes them much faster with the rest like reduction ops on float32 [56].
- quantization-aware training, involves clamping and rounding floating-point values during training to simulate int8 precision[57].
- using LoRA (Low-Rank Adaptation) and its variants which uses lower rank matrices of the matrix multiplication layers i.e. linear layers [58].

Of the common training techniques mentioned, we'll instead focus on Data Distributed Parallel, Fully Sharded Data Parallel, reduced precision training, and optimizing the model graph using Jax. Summarily, we'll focus on scalable multi-GPU and TPU training. The compute for these techniques will be remotely spawned with the much needed GPU RAM and tunneled via ssh.

Remote Compute

For this section, the platforms *RunPod* and *Vast* are to be used for spawning the compute needed, you can choose either of these for your workloads, but now for the connection, ssh is the just needed tool for connecting and running commands and programs in the compute.

What is Secure Shell (SSH)?

This is a secure protocol that enables logging into remote compute, running commands, copying files to and from the compute, and installing tools. Think of it as a way to always use your normal computer via the terminal and not by using Graphical Interfaces[59].

[56] Automatic Mixed Precision
PyTorch blog by Michael Carilli, Created 2020, Updated 2025

[57] Quantization
Quantization Aware Training for Static Quantization

[58] Fine-Tuning Llama2 with LoRA

[59] Well, you could use graphical interfaces, but by port forwarding, and that is beyond the scope of this article.

Spawn a GPU Compute in RunPod

The cited article[60] goes into generating an ssh key, setting up the public key in the platform, then ssh-ing into the spawned remote compute. I'd recommend two great tools that will help navigate between your local and remote compute with great flexibility

- helix editor[61], an terminal-based text editor that does not need customizations by having to write configs in a complex functional language. Neat for and editing programs and writing automation tools within the remote compute.
- tmux[62], a tool that helps in managing multiple sessions, local and remote, without having to switch terminals or apps. Great for terminal-based multi-tasking and persistent ssh tunneling.

Going into runpod, I need the *A40, 48GB VRAM* pod. This allows for inference given no parallelism. Next, as per specified in the benchmark of reference[63], we'll upgrade to a compute of approximately *40GB* per gpu, 8 counts of such.
Runpod gives us this compute for $0.4/hour, a nice option considering other options like Vast.ai gives us the same for $0.471/hour, not much difference for small training, but considering days of training, becomes a significant diference.
After moving all necessary files[64] to the spawned remote compute using the command

```
scp -P $PORT {core_utils,train_official}.py
    root@$IP:/root/
```

The time per epoch hours attained is

```
time : 0.33440 hours per epoch
```

or to say it another way, 20 minutes. However, one thing is to be noted from ViT benchmarks for the *ViT-L/16*, the global batch size is 512, meaning for the 8 optimal gpus used, the batch size per gpu then becomes 64, so, runnning another epoch for the now modified batch size of 64 gives the time per epoch of

```
time : 0.32292 hours per epoch
```

The next section then goes into the start of parallelism and how to beat the time achieved by Google (or approximate it) of

```
time : 0.00722251 hours per epoch
```

[60] Use SSH

[61] Helix Editor Official Site

[62] Tmux Getting Started

[63] Benchmark Table

Model	Framework	Accelerator	Global batch-size	Precision	Img/sec	Time in hrs per epoch (SDK images)	Per hour machine cost (USD) for Vertex AI (europe-west4)	Cost (USD) per epoch on Vertex AI
ViT-L16 (300M)	PyTorch Multi GPU with DDP strategy	8 A100-40GB (1 host)	512	float16	1923	0.00722251	34.482189	0.249
	JAX TPU	TPU v3 8 cores	512	bfloat16	760	0.01851851	10.12	0.1874
	JAX TPU POD	TPU v3 32 cores (4 hosts)	2048	bfloat16	3020	0.00459896	36.8	**0.1692**
	JAX GPU	1 A100	128	bfloat16	296	0.04692192	4.310274	0.2022
	JAX Multi GPU	8 A100-40GB (1 host)	1024	bfloat16	2213	0.00627604	34.482189	0.2164
ViT-H14 (660M)	PyTorch Multi GPU with DDP strategy	8 A100-40GB (1 host)	128	float16	552	0.02516103	34.482189	0.8676
	JAX TPU POD	TPU v3 32 cores (4 hosts)	1024	bfloat16	986	0.01408609	36.8	**0.5183**
	JAX Multi GPU	8 A100-40GB (1 host)	256	bfloat16	781	0.01778346	34.482189	0.6132
ViT-g14 (1B)	PyTorch Multi GPU with DDP strategy	8 A100-40GB (1 host)	128	float16	408	0.03404139	34.482189	1.1738
	JAX TPU POD	TPU v3 32 cores (4 hosts)	512	bfloat16	579	0.02398771	36.8	**0.8827**
	JAX Multi GPU	8 A100-40GB (1 host)	128	bfloat16	427	0.03252667	34.482189	1.1215
ViT-G14 (1.8B)	PyTorch Multi GPU with Deepspeed ZeRO Stage3 strategy	8 A100-40GB (1 host)	256	float16	195	0.07122507	34.482189	2.4559
	JAX TPU POD with FSDP	TPU v3 32 cores (4 hosts)	4096	bfloat16	333	0.04170837	36.8	**1.5348**
	JAX Multi GPU with FSDP	8 A100-40GB (1 host)	256	bfloat16	295	0.04708097	34.482189	1.6234

[64] the files can be found in the repository and the folder https://github.com/Marvin-desmond/ScalingViTsAcrossTrainingCompute/blob/main/transformerViT/

Message Passing Interface (MPI)

As adapted from the book, Programming Massively Parallel Processors[65], a MPI is

a programming interface in which computing nodes in a cluster do not share memory. This memory isolation strategy hence dictates that all data sharing and interaction within must be done through explicit message passing, as common in High Performance Computing(HPC). In HPC, apps written in MPI have run successfully on cluster computing systems with more than 100,000 nodes. Due to this high number of nodes and lack of shared memory, the amount of effort then that is needed to port an application into MPI can be quite high across computing nodes.

This tool is commonly implemented in C, with its Python ported version[66] to be used by high-level compute developers. PyTorch implements all this in Data Distributed Parallel which has been tuned for multi-GPU hence is much much faster, one that is part of this article that is coming after this. However, using MPI natively gives more control.

After installing your version of MPI[67], then compiling it will be by using *mpicc* instead of *gcc*. This *hello world* code of MPI in C

```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
  MPI_Init(&argc, &argv);
  int name_len, world_size;
  MPI_Comm_size(MPI_COMM_WORLD, &world_size);
  char processor_name[MPI_MAX_PROCESSOR_NAME];
  MPI_Get_processor_name(processor_name, &name_len);
  char *s_or_p_processor = world_size < 2 ? "processor" :
       "processors";
  printf("Hello world from processor %s out of %d %s\n",
   processor_name, world_size, s_or_p_processor);
  MPI_Finalize();
}
```

thus when compiled gives

```
> mpicc -o hello_mpi hello_mpi.c && ./hello_mpi
Hello world from processor Marvins-MacBook-Pro-4.local
    out of 1 processor
```

[65] Programming Massively Parallel Processors
A Hands-on Approach
4th Edition - May 28, 2022
Buy Link

[66] mpi4py

[67] https://www.open-mpi.org/software/ompi/v5.0/

So knowing that MPI uses multiprocessing, multiple processes are spawned, each of these processes having their own memory. This then provides parallelism as these processes are independent of each other and do not have to wait for one another, executing across multiple input values as the input data is distributed across processes.

Data Parallelism

From the context of model training, considering you have a very large dataset, then data parallelism means that you take your model and copy it across multiple machines (GPUs), then different non-overlapping batches of data are uniquely sent across the different machines, forward pass done in each machine, gradients locally computed, then the computed gradients are then aggregated across all processes, then averaged on a master node by the number of gpus to to give global gradients, before the processes are sent the new global gradients that then are used to update the models on each of those machines terms of their parameters. This ensures that all models are thus a copy of each other.

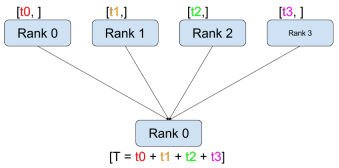
From this, then two collective communication strategies are key

- reduce (or all-reduce) [68]
- broadcast [69]

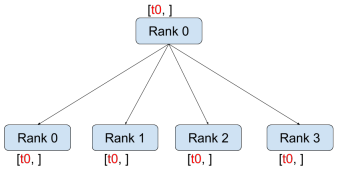
Let's consider an array with 4 values representative of four batches, and so I send the values to the four processes[70].

```c
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
    MPI_Init(&argc, &argv);
    int rank, world_size, scattered_val;
    int values[4] = {39, 72, 129, 42};
    MPI_Comm_size(MPI_COMM_WORLD, &world_size);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Scatter(&values, 1, MPI_INT, &scattered_val, 1,
        MPI_INT, 0, MPI_COMM_WORLD);
    printf("Processor %d received %d\n",rank,
        scattered_val);
    MPI_Barrier(MPI_COMM_WORLD);
    MPI_Finalize();
}
```

[68] reduce ~ computes a reduction operation then stores the result in a master node, all-reduce instead stores the result in all the processes



[69] broadcast ~ copies the computed global gradient from the master process to the other processes.



diagrams courtesy of *Writing Distributed Applications with PyTorch*

[70] and run the program as

```
> mpicc -o hello_mpi hello_mpi.c
> mpirun -np 4 ./hello_mpi
Processor 0 received 39
Processor 1 received 72
Processor 2 received 129
Processor 3 received 42
```

the MPI barrier is since the forward and backward pass for each process needs to finish and all local gradients sent to the master process, so it synchronizes all processes upto when the last process sends the local gradient to the master node.

Simple Reduce and Broadcast

Right before the line *MPI_Finalize()*, consider that as the starting point. Assuming each process involves computation that simulates the gpu computation of the forward and backward pass, which I then gather the results to a master process, then the additional code is [71]

```
    // ...
    //a computation to simulate a forward and back pass
    scattered_val = scattered_val * 0.5;
    printf("Processor %d updated value %d\n",rank,
        scattered_val);
    MPI_Barrier(MPI_COMM_WORLD);
    // gather to rank zero
    int *rbuf;
    if (rank == 0) {
        rbuf = (int *)malloc(world_size*sizeof(int));
    }
    MPI_Gather(&scattered_val, 1, MPI_INT, rbuf, 1,
        MPI_INT, 0, MPI_COMM_WORLD);
    if (rank == 0){
        for (int i=0; i < world_size; i++) {
            printf("Rank %d: rbuf[%d] = %d\n", rank, i,
                rbuf[i]);
        }
        free(rbuf);
    }
    //...
```

However, I need not to do a gather, but a reduce, so then doing a reduce with MPI leads to the above code being modified, from the line *int *rbuf*, as

```
// ...
// gather to rank zero
int global_avg;
MPI_Reduce(&scattered_val, &global_avg, 1, MPI_INT,
    MPI_SUM, 0, MPI_COMM_WORLD);
if (rank == 0){
     printf("Rank %d: sum %d average %.1f\n",
      rank, global_avg, (float)global_avg/world_size);
}
// ...
```

```
Rank 0: sum 140 average 35.0
```

[71] the result of the program is thus

```
> mpicc -o hello_mpi hello_mpi.c
> mpirun -np 4 ./hello_mpi
Processor 0 received 39
Processor 0 updated value 19
Processor 1 received 72
Processor 1 updated value 36
Processor 2 received 129
Processor 2 updated value 64
Processor 3 received 42
Processor 3 updated value 21
Rank 0: rbuf[0] = 19
Rank 0: rbuf[1] = 36
Rank 0: rbuf[2] = 64
Rank 0: rbuf[3] = 21
```

Now let's broadcast the resulting average value, signifying the computed global gradients, to all the processes (nodes)[72].

```
// ...
// Broadcast the result to all the processes
float broadcast_val = 0.0f;
if (rank == 0){
  broadcast_val = (float)global_avg/world_size;
}
MPI_Bcast(&broadcast_val, 1, MPI_FLOAT, 0,
    MPI_COMM_WORLD);
printf("Processor %d final value %f\n",rank,
    broadcast_val);
// ...
```

We actually don't need *MPI_Barrier* before the collective operations since they implicitly require synchronization before starting to execute.

MPI in Python

Considering the first speedup of ViT training will use this library, *mpi4py*, let us rewrite the previous implementation of the reduce and broadcast in Python, with no need for explanations as it does the same operations[73].

```
from mpi4py import MPI
import numpy as np
comm = MPI.COMM_WORLD
size, rank = comm.Get_size(), comm.Get_rank()
if rank == 0:
    data = [39, 72, 129, 42]
else:
    data = None
data = comm.scatter(data, root=0)
print(f"Processor {rank} received {data}")
comm.Barrier()
data = data * 0.5
print(f"Processor {rank} updated {data:.2f}")
resulting_sum = np.array(0.0,dtype=np.float64)
comm.Reduce(
        np.array(data, dtype=np.float64),
        resulting_sum, op=MPI.SUM, root=0)
if rank == 0:
    print(f"Processor {rank} sum {resulting_sum:.2f}")
data = comm.bcast(resulting_sum/size, root=0)
print(f"Processor {rank} final {data:.2f}")
```

[72] the result of the program is

```
Processor 0 received 39
Processor 1 received 72
Processor 2 received 129
Processor 3 received 42
Processor 3 updated value 21
Processor 3 final value 35.000000
Processor 2 updated value 64
Processor 2 final value 35.000000
Processor 0 updated value 19
Rank 0: sum 140 average 35.0
Processor 0 final value 35.000000
Processor 1 updated value 36
Processor 1 final value 35.000000
```

[73] and the Python equivalent program using MPI is run as *ensure mpi4py is installed using pip install mpi4py*

```
mpiexec -n 4 python hello_parallel.py
```

which gives the expected result as

```
Processor 0 received 39
Processor 2 received 129
Processor 3 received 42
Processor 1 received 72
Processor 1 updated 36.00
Processor 3 updated 21.00
Processor 0 updated 19.50
Processor 2 updated 64.50
Processor 0 sum 141.00
Processor 0 final 35.25
Processor 2 final 35.25
Processor 1 final 35.25
Processor 3 final 35.25
```

DDP, a message passsing tool for multi-node GPUs

So, I am going to skip delving into mpi4py with torch and training (for now), because I need to build torch from scratch for MPI to work for GPUs, and the last time I tried to build a tool[74], I did not like the patience I had to endure for it to complete.

Distributed Data Parallel is a tool that does distributed computations for pipelines by assigning accelerators for the said computations and also facilitates the communication between different processes which can either be peer-to-peer communication or collective communications.

PyTorch, using the distributed package, creates a group of processes that are "device-aware" using the *torch.distributed.init_process_group*, hook them up with fast communication backends, *nccl*, *gloo* and mpi, then prepare your data pipeline and model implementation to work in this multi-process context. Based on this then, a few environment variables are used to glue everything together,

- **world_size** ∼ total number of GPUs in your cluster
- **rank** ∼ the unique id of a GPU.
- **store** ∼ a shared key-value store used for initializing the distributed process group by exchanging information like addresses and ports.
- **process group** ∼ a subset of processes(GPUs) that communicate with each other. Default group includes all GPUs.

For CPU, backend to be used is *gloo* with the maximum world size being the available physical CPU cores, though it is not recommended to use all the cores as this may degrade performance. Making sure each process has the capability to communicate to each other can be done with

```
import os, sys, torch.distributed as dist
import torch.multiprocessing as mp
def init_process(rank,size,fn,backend="gloo"):
    os.environ['MASTER_ADDR'] = '127.0.0.1'
    os.environ['MASTER_PORT'] = '29500'
    dist.init_process_group(
        backend,rank=rank,world_size=size)
    fn()
    dist.barrier()
    dist.destroy_process_group()
```

[74] Neuron ∼ an inference-efficient compute tool
by Marvin, June 2023 Article

Spawning processes using torch.multiprocessing

With the communication between processes defined, spawning 4 processes is then done with [75]

```
def run():
    rank = dist.get_rank()
    size = dist.get_world_size()
    print(f"rank {rank} size {size}")
if __name__ == "__main__":
    world_size = 4 # os.cpu_count()
    mp.set_start_method("spawn")
    mp.spawn(fn=init_process, args=(world_size,run),
        nprocs=world_size, join=True)
```

Rewriting the previous implementations of collective communications in C and Python now in *torch.distributed*, the resulting code is[76]

```
import torch
def run(rank,size):
    tensor = torch.zeros(1)
    data = [39,72,129,42]
    tensor = torch.tensor([data[rank]],
        dtype=torch.float32)
    print(f"rank {rank} size {size} data {tensor}")
    dist.barrier() # for print convenience
    tensor = tensor * 0.5
    print(f"rank {rank} updated data to {tensor}")
    dist.barrier() # for print convenience
    # reduce op
    dist.reduce(tensor,0,dist.ReduceOp.SUM)
    if rank == 0:
        print(f"rank {rank} reduced value {tensor}")
    # broadcast the average
    if rank == 0:
        tensor = tensor / size
    dist.broadcast(tensor,src=0)
```

Note that *reduce* and *broadcast* can be reduced to *all_reduce* as

```
    dist.all_reduce(tensor,dist.ReduceOp.SUM)
    tensor = tensor / size
    print(f"rank {rank} final value {tensor}")
```

The reason for being redundant was to show how collective communication ops works for the different tools that are common.

[75] how spawn works is very interesting, it calls the function *init_process* as *init_process(i, *args)* where i is the process index/rank. This then means I don't need to pass the rank argument as needed by the *init_process*. Also, I can either pass rank and world_size to the run function or use the *dist.get_rank()* and *dist.get_world_size()* for the variables, whichever works for you.

[76] output of Python code

```
rank 3 size 4 data tensor([42.])
rank 3 updated data to tensor([21.])
rank 3 final value tensor([35.2500])
rank 1 size 4 data tensor([72.])
rank 1 updated data to tensor([36.])
rank 1 final value tensor([35.2500])
rank 2 size 4 data tensor([129.])
rank 2 updated data to tensor([64.5000])
rank 2 final value tensor([35.2500])
rank 0 size 4 data tensor([39.])
rank 0 updated data to tensor([19.5000])
rank 0 reduced value tensor([141.])
rank 0 final value tensor([35.2500])
```

Distributing batches to different GPUs

This is the time to go back to your cloud GPU platform i.e. RunPod, and spin up an instance of 2 gpus. Based on the number of gpus, I compute the datasets per rank. In doing this, first of all, I rewrite the dataset initializer into a function

```
def create_data():
    train_data = torchvision.datasets.CIFAR10(
      root="./datasets", train=True, transform=transforms,
           download=True)
    test_data = torchvision.datasets.CIFAR10(
      root="./datasets", train=False, transform=transforms,
           download=True)
    return (train_data,test_data)
```

And so, the next thing is to partition the dataset for each gpu (rank). Given I provisioned 2 A40 gpus, each with VRAM 48GB, then to get local batch size of 32, I set the global batch as 64.

```
BATCH = 64
bsz = BATCH // size
```

Now with the local batch size, let's split the train and test datasets for each gpu.

```
train_data,test_data = create_data()
fracs = [1.0 / size for _ in range(size)] # [0.5,0.5]
gen = torch.Generator().manual_seed(SEED)
train_splits = random_split(train_data, fracs, generator=gen)
test_splits = random_split(test_data, fracs, generator=gen)
part_train = train_splits[rank]
part_test = test_splits[rank]
```

and so then, I can proceed to create the data loaders for both train and test which is unique to each gpu in the host.

```
create_loader=lambda data,batch: DataLoader(data,batch,True)
part_train_loader = create_loader(part_train, bsz)
part_test_loader = create_loader(part_test, bsz)
```

and hence the code above forms the partition dataset implementation[77]. Knowing this, running the partition dataset function will only be run on that process which will then pick the partition to be loaded to a specific gpu of id rank. Using the same seed ensures the reproducibility in global and uniqueness in local batches across the device-aware processes.

The next section hence goes into initializing copies of the model for each rank, then training the copies on each data partition before I compute the average of the gradients using the collective communication *all_reduce*[78].

[77]

```
def partition_dataset(rank,size):
    train_data,test_data = create_data()
    bsz = BATCH // size
    fracs = [1.0/size for _ in range(size)]
    gen =
         torch.Generator().manual_seed(SEED)
    train_splits = random_split(
        train_data, fracs, generator=gen)
    test_splits = random_split(
        test_data, fracs, generator=gen)
    p_train = train_splits[rank]
    p_test = test_splits[rank]
    ptr_loader = create_loader(p_train, bsz)
    pts_loader = create_loader(p_test, bsz)
    return (ptr_loader,pts_loader,bsz)
```

[78] ensure that the backend for the processes is at this point set to *nccl* for gpu nodes.

Army of ViT-L/16's on the GPUs

Creating a new function for training the army of models, let's first get the device for that rank using

```
device = torch.device(f"cuda:{rank}")
```

So for each rank, the model is initialized as[79]

```
model = create_model()
optimizer = torch.optim.SGD(
    model.parameters(),lr=1e-3,momentum=.9)
```

Then, getting the number of batches per rank is derived using

```
num_batches = ceil(len(local_train_loader.dataset) //
    float(bsz))
```

and so the single gpu training code only now has a single line update to

```
epoch_loss = 0.0
for i, (images, labels) in enumerate(part_train_loader):
    images = images.to(device)
    actual = labels.to(device)
    optimizer.zero_grad()
    predicted = model(images)
    loss = criterion(predicted,actual)
    epoch_loss += loss.item()
    loss.backward()
    average_gradients(model)
    optimizer.step()
```

With the great understanding of collective communication as at of now, average gradients takes all gradients computed by *loss.backward()*, averages them and broadcasts them, all in one using the *all_reduce*.

```
def average_gradients(model):
    size = float(dist.get_world_size())
    for param in model.parameters():
        dist.all_reduce(param.grad.data,
            op=dist.ReduceOp.SUM)
        param.grad.data /= size
```

With these changes in mind, what speed ups do we get from single A40 GPU training to training on 2 gpus, batch size 32?[80].

[79] with the *create_model* function being

```
def create_model():
    vit_l_16 = VisionTransformer(L16Config)
    vit_l_16 = vit_l_16.to(device)
    vit_l_16.train()
    return vit_l_16
```

[80] the complete code for multi-GPU training is at https://github.com/Marvin-desmond/ScalingViTsAcrossTrainingCompute/blob/main/transformerViT/multi_gpu_train_pipeline.py

Training on 2 GPUs

For the batch size 32, the resulting time per epoch hours begets[81]

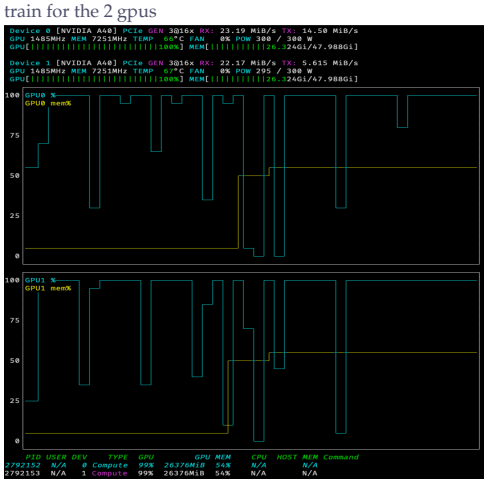
```
rank 1 time : 0.20232 hours per epoch
rank 0 time : 0.20232 hours per epoch
```

As can be seen, training on the new pipeline reduced the time from *20 minutes* to *12 minutes* for the batch size 32, and the time is further reduced to 11 minutes as can be seen below

```
rank 0 time : 0.17932 hours per epoch
rank 1 time : 0.17929 hours per epoch
```

for a batch size of 64, still a long way to go. The loss reduces as is expected and after 2 epochs the resulting accuracy is 31%, up from a random baseline of 8%.

[81] nvtop tool showing the interesting shift from inference to train for the 2 gpus



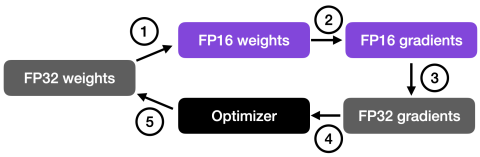
Reduced Float Precision Training

By default, PyTorch initializes weights and biases as 32-bit floating point values. Of course, a larger number of bits corresponds to a higher precision, which lowers the chance of errors accumulating during computations. However, in deep learning, because it has been computationally expensive, 32 bits has then been adopted. GPU hardware is also not optimized for 64-bit floating point operations.

Given this, then the earlier training used float32 for the floating point operations. Let us then go into lower memory footprint during training by doing reduced float precision training for the model. However, this reduction in precision can be tricky since it might cause underflows and instabilities due to issues such as vanishing or exploding gradients that can occur when using lower-precision arithmetic. This then introduces us to two tools, *torch.autocast* whose instance of a context manager runs regions of your script in mixed precision.

In such regions, computation ops on the set device run in a dtype chosen by autocast to improve performance while maintaining accuracy. This dtype would now be float16, with the gradients then computed in float32 for numerical stability. Also, Another tool, *GradScaler* scales gradients to prevent underflowing[82].

[82] forward and backward pass floating point precision changes



Implementing Mixed precision Training

Let's implement torch.autocast to reduce floating point ops in the layers to float16 while maintaining sensitive layers i.e. *LayerNorm, loss values* to float32. With loss values in float32, gradient computation uses higher floating point values hence better accuracy in convergence.

```
with torch.autocast(
    device_type=device, dtype=torch.float16):
    predicted = model(images)
    assert predicted.dtype is torch.float16
    loss = criterion(predicted,actual)
    assert loss.dtype is torch.float32
```

Let's now define the GradScaler to scale the gradients and perform gradient updates conveniently, only doing so when there's no NaN's or infs.

```
scaler = torch.amp.GradScaler(device)
# the above code ...
scaler.scale(loss).backward()
average_gradients(model)
scaler.step(optimizer)
scaler.update()
optimizer.zero_grad()
```

Time per epoch hours then optimizes this training to

```
rank 0 time : 0.11699 hours per epoch
rank 1 time : 0.11732 hours per epoch
```

approximately 7 minutes for the new pipeline.
Note that doing *model.half()* trains in 4 minutes but then it comes with instabilities of sensitive layers with loss values and gradient computations being in float16. This results in accuracy after two epochs being 28.94% versus 32.68% for mixed precision training.

2 H100's over A40's

Upgrading the gpus from the A40s to the H100s gives me

```
rank 0 time : 0.03912 hours per epoch
rank 1 time : 0.03906 hours per epoch
```

which when scaled approximately linearly for 8 gpus, would give 0.00978 of an hour, closer to the realized time. But the Google benchmarks only use the A100-40GB, so that would be "cheating", but we can take that.

Fully Sharded Data Parallel

In constrast to data parallelism where model replica is stored in every device process across the multiple processes, fully sharded data parallelism shards the model parameters, the gradients and optimizer states[83] and scatters them across the gpus. This mode is used in training the large ViT-G/14 whose replica cannot be trained on a single GPU and hence needs sharding on many GPUs, offloading GPU memory. Google DeepMond uses 256 as the global batch meaning the sharded model across the GPU processes use 32 as the local batch size. This package is in *torch.distributed.fsdp*.

In this mode of parallelism, I should shard the submodules as well as the root model[84], again noting that the backend should be *nccl*.

```
from torch.distributed.fsdp import fully_shard,
    FSDPModule
def apply_fsdp():
    vit_l_16 = VisionTransformer(L16Config)
    for vit_block in vit_l_16.vit_blocks:
        fully_shard(vit_block)
    fully_shard(vit_l_16)
    assert isinstance(vit_l_16, VisionTransformer)
    assert isinstance(vit_l_16, FSDPModule)
    print(vit_l_16)

if __name__ == "__main__":
    world_size = torch.cuda.device_count()
    mp.set_start_method("spawn")
    mp.spawn(fn=init_process,
        args=(world_size,apply_fsdp), nprocs=world_size,
        join=True)
```

Now, on checking the parameters being now sharded, their types change from *Tensor* to *DTensor*[85].

```
    # within apply_fsdp function ...
    from torch.distributed.tensor import DTensor, Shard
    param = next(iter(vit_l_16.parameters()))
    print(type(param))
```

DTensor in this case represents the sharded parameters. Now that our model has been sharded, let us develop the training pipeline for FSDP.

[83] Getting Started with Fully Sharded Data Parallel (FSDP2)
Feng et al. 2022, updated May 2025

[84] the output for the sharded model begets

```
FSDPVisionTransformer(
    (image_embeddings): ImageEmbeddings(
        (conv_then_project): Conv2d(3,
            1024, kernel_size=(16, 16),
            stride=(16, 16))
    )
    (vit_blocks): Sequential(
        (0): FSDPViTBlock(
    ...
```

[85] the output for the type begets

```
<class 'torch.distributed.tensor.DTensor'>
<class 'torch.distributed.tensor.DTensor'>
```

Sharded data by way of DistributedSampler

DistributedSampler passed to the dataLoader loads onto the given process the data subset unique to it. Let's understand a bit more on this by building a very simpler data loader. Taking an ideal y for a given x distribution and building a torch dataset, then I have.

```
x = torch.arange(10,dtype=torch.float32)
y = x ** 2 # usually the output is noisy
data = TensorDataset(x,y)
```

Printing a subset of our Dataset gives us an idea of what the data looks like. Of course, by now you know it prints three times unless you have a conditional for which process the print whould be in. Given it is still non-unique, all the processes print the same data subset.

```
print(data[:5])
```

```
(tensor([0., 1., 2., 3., 4.]), tensor([ 0.,  1.,  4.,  9., 16.]))
(tensor([0., 1., 2., 3., 4.]), tensor([ 0.,  1.,  4.,  9., 16.]))
(tensor([0., 1., 2., 3., 4.]), tensor([ 0.,  1.,  4.,  9., 16.]))
```

Assuming we have three running processes, then our sampler reflects that in the *num_replicas* argument.

```
sampler =
    DistributedSampler(data,rank=rank,num_replicas=size)
```

And now we can pass our data, sampler and batch size among other processing optimized parameters i.e. number of workers to the *DataLoader*.

```
loader = DataLoader(data,sampler=sampler,batch_size=2)
```

This now gives us each process having 2 batches, each batch having two samples. Think again! Total data is ten samples, split three ways, gives four samples per rank, understanding that two values are repeated because we didn't drop the fractional part of the dataset hence rounding up occurs i.e. *drop_last* is set to *False*. Printing the two batches per rank will give unique samples, except of course the two repeated ones[86].

```
for x,y in loader:
    print(f"rank {rank} data : {x = }")
```

[86] the result of the simple distributed sampler gives

```
rank 0 data : x = tensor([4., 5.])
rank 1 data : x = tensor([1., 3.])
rank 2 data : x = tensor([7., 9.])
rank 0 data : x = tensor([0., 2.])
rank 1 data : x = tensor([8., 4.])
rank 2 data : x = tensor([6., 1.])
```

I have written this without the multiprocessing part because that has been explored in-depth and you can reproduce three processes for backend *gloo* for your local cpu workflows.

A tiny bit more...

One more necessary thing i'd like to add, due to the distributed sampling, shuffling might be a problem for multiple epochs of training, so a necessary line of code is needed so it always shuffles.

```
sampler = DistributedSampler(
    data,rank=rank,num_replicas=size,shuffle=True
    )
loader = DataLoader(data,sampler=sampler,batch_size=2)
for epoch in range(2):
    for x,y in loader:
        if rank == 0:
            print(f"rank {rank} data : {x = }")
```

As can be noted, shuffling is set to true but it prints the same data batches for the two epochs.[87]Correcting it is done by the code added as can be seen below[88]

```
    for epoch in range(2):
        sampler.set_epoch(epoch)
        for x,y in loader:
# ...
```

And hence now, the cifar10 pipeline for the fsdp model is concretely implemented using distributed sampling as shown below, with parameters I've gone through

```
def partition_dataset(rank,size,batch_size):
    train_data,test_data = create_data()
    sampler1 = DistributedSampler(train_data,
    rank = rank, num_replicas = size, shuffle = True)
    sampler2 = DistributedSampler(
        test_data,
        rank = rank, num_replicas = size)
    train_kwargs = {'batch_size': batch_size,
                    'sampler': sampler1}
    test_kwargs = {'batch_size': batch_size,
                    'sampler': sampler2}
    cuda_kwargs = {'num_workers': 2, 'pin_memory': True,
    'shuffle': False}
    train_kwargs.update(cuda_kwargs)
    test_kwargs.update(cuda_kwargs)
    train_loader = create_loader(train_data,train_kwargs)
    test_loader = create_loader(test_data,test_kwargs)
    return (
        train_loader, sampler1, test_loader, sampler2)
```

[87] before the shuffling fix, the batches for the two epochs print

```
rank 0 data : x = tensor([4., 5.])
rank 0 data : x = tensor([0., 2.])
rank 0 data : x = tensor([4., 5.])
rank 0 data : x = tensor([0., 2.])
```

[88] adding the line of code now fixes shuffling

```
rank 0 data : x = tensor([4., 5.])
rank 0 data : x = tensor([0., 2.])
rank 0 data : x = tensor([5., 2.])
rank 0 data : x = tensor([9., 4.])
```

The train function as always

The train does not change much actually, apart from the tqdm for progress bar monitoreed for the master process, the rest of the code remains the same

```
def train(model, train_loader, test_loader,
          optimizer, criterion, bsz, sampler=None):
    rank, size = dist.get_rank(), dist.get_world_size()
    EPOCHS = 2
    for EPOCH in range(EPOCHS):
        if sampler:
           sampler.set_epoch(EPOCH)
        if rank==0:
            inner_pbar = tqdm(
             range(len(train_loader)),
             colour="blue", desc="r0 Training Epoch")
        epoch_loss = 0
        for images,labels in train_loader:
            images = images.to(rank)
            labels = labels.to(rank)
            predicted = model(images)
            loss = criterion(predicted,labels)
            epoch_loss += loss.item()
            if rank==0:
                inner_pbar.update(1)
            loss.backward()
            optimizer.step()
            optimizer.zero_grad()
```

And then finally, the program that stitches every defined function[89]is then developed as shown below, with the batch per rank being 16 for one to train *ViT-G/14* on the 8 *A100-40GB VRAM*.

```
BATCH=16
def train_fsdp(rank,size):
    fsdp_model = apply_fsdp(rank,size)
    (train_loader, sampler1,test_loader, sampler2
    ) = partition_dataset(rank,size,BATCH)
    optimizer = torch.optim.SGD(
                    fsdp_model.parameters(),lr=1e-3,
                    momentum=.9)
    loss_fn = torch.nn.CrossEntropyLoss().to(rank)
    train(fsdp_model, train_loader, test_loader,
          optimizer, loss_fn, BATCH, sampler1)
```

[89] the *apply_fsdp* is now neatly defined as

```
def apply_fsdp(rank,size):
    """update as needed to G/14 model"""
    vit_l_16 = VisionTransformer(L16Config)
    for vit_block in vit_l_16.vit_blocks:
        fully_shard(vit_block)
    fully_shard(vit_l_16)
    return vit_l_16
```

[90]with the

The train function as always

[91] with the