<u>TensorFlow Transformer Tutorial</u> (<u>https://www.tensorflow.org/text/tutorials/transformer)</u>

We will take a look at the actual code of a Transformer.

There are many pieces, which we will examine individually.

We will proceed starting with a high level view and descend to a lower level

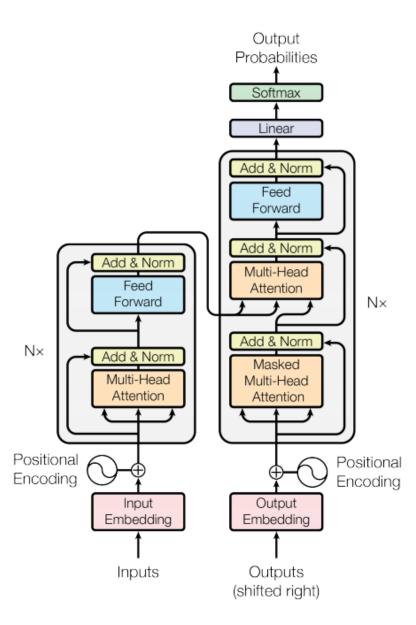
means reading the code from bottom to top

There are many subtle points which we will highlight with the tag **SUBTLETY**

One of the key components of a Transformer is the Attention mechanism.

In the code we examine, the base Attention class is via a MultiHeadAttention layer type

- we will study this layer separately
- so as not to distract from the other details of the Transformer architecture



<u>The Model: Transformer</u> (<u>https://www.tensorflow.org/text/tutorials/transformer#the_transformer</u>)

WHERE ARE THE RESISUAL CONNECTIONS AND ADD/NORM ??? Built into the lower level objects ??*

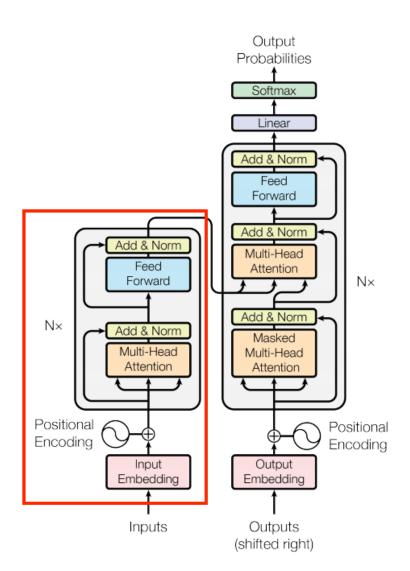
- The Transformer is a Model: a subclass of tf.keras.Model
- The initializer creates
 - An Encoder
 - A Decoder
 - a final_layer which converts the vector at each position into logits over the distribution of tokens

The model overrides the call method

- defines what happens when we pass an input to the Transformer
- passes the contextinput to the Encoder
- the Encoder output is passed to the Decoder
- the Decoder output (logits) is passed through a layer to produce a logit (at each position)

```
def call(self, inputs):
       # To use a Keras model with `.fit` you must pass all your inputs in the
       # first argument.
        context, x = inputs
       context = self.encoder(context) # (batch_size, context_len, d_model)
       x = self.decoder(x, context) # (batch_size, target_len, d_model)
       # Final linear layer output.
        logits = self.final_layer(x) # (batch_size, target_len, target_vocab_s
ize)
        try:
          # Drop the keras mask, so it doesn't scale the losses/metrics.
         # b/250038731
          del logits._keras_mask
        except AttributeError:
          pass
```

<u>The Encoder</u> (<u>https://www.tensorflow.org/text/tutorials/transformer#the_encoder_layer</u>)



Confusion warning

The Encoder object is the stack of encoder blocks (which are called EncoderLayer 's)

The Encoder is a Layer: sub-class of tf.keras.layers.Layer)

- The initializer creates the sub-components of the Encoder
 - Positional Embedding
 - A sub-component (confusingly named EncoderLayer) which is an array of blocks whose elements are objects containing
 - Self-Attention
 - Feed-forward network
 - This array (of length num_layers) is the stack of blocks

The call method defines how the layer behaves when presented with input

- calls the Positional Embedding on the Encoder input
- passes the result to the stacked EncoderLayer's
 - Self-Attention followed by Feed Forward

```
def call(self, x):
    # `x` is token-IDs shape: (batch, seq_len)
    x = self.pos_embedding(x)  # Shape `(batch_size, seq_len, d_model)`.

# Add dropout.
    x = self.dropout(x)

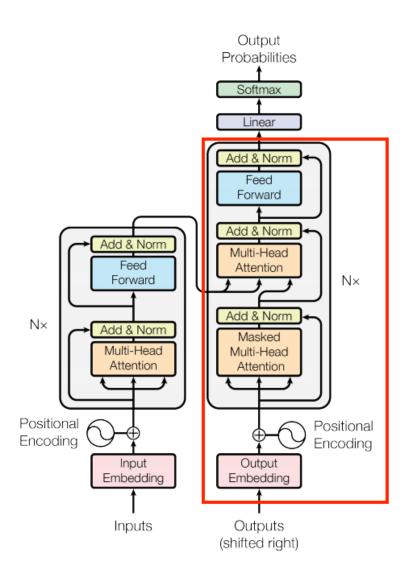
for i in range(self.num_layers):
    x = self.enc_layers[i](x)

return x  # Shape `(batch_size, seq_len, d_model)`.
```

The EncoderLayer

- initializer creates sub-components
- the call method is over-ridden to pass inputs through the sub-components

<u>The Decoder</u> (https://www.tensorflow.org/text/tutorials/transformer#the_d ecoder)



Confusion warning

The Decoder object is the *stack* of decoder blocks (which are called DecoderLayer 's)

The Decoder is a Layer: sub-class of tf.keras.layers.Layer)

- The initializer creates the sub-components of the Decoder
 - Positional Embedding
 - A sub-component (confusingly named DecoderLayer) which is an array of blocks whose elements are objects containing
 - Self-Attention
 - Cross-Attention
 - Feed-forward network
 - This array (of length num layers) is the *stack* of blocks

The call method defines how the layer behaves when presented with input

- calls the Positional Embedding on the Decoder input
- passes the result to the stacked DecoderLayer's
 - Causal Self-Attention followed by
 - Cross-Attention followed by Feed Forward

```
def call(self, x, context):
    # `x` is token-IDs shape (batch, target_seq_len)
    x = self.pos_embedding(x) # (batch_size, target_seq_len, d_model)

x = self.dropout(x)

for i in range(self.num_layers):
    x = self.dec_layers[i](x, context)

self.last_attn_scores = self.dec_layers[-1].last_attn_scores

# The shape of x is (batch_size, target_seq_len, d_model).
return x
```

The DecoderLayer

• initializer creates sub-components

```
class DecoderLayer(tf.keras.layers.Layer):
  def __init__(self,
               d model,
               num_heads,
               dff,
               dropout_rate=0.1):
    super(DecoderLayer, self).__init__()
    self.causal_self_attention = CausalSelfAttention(
        num_heads=num_heads,
        key_dim=d_model,
        dropout=dropout_rate)
    self.cross_attention = CrossAttention(
        num_heads=num_heads,
        key_dim=d_model,
        dropout=dropout_rate)
    self.ffn = FeedForward(d_model, dff)
```

The call method is over-ridden to pass inputs through the sub-components

```
def call(self, x, context):
    x = self.causal_self_attention(x=x)
    x = self.cross_attention(x=x, context=context)

# Cache the last attention scores for plotting later
    self.last_attn_scores = self.cross_attention.last_attn_scores

x = self.ffn(x) # Shape `(batch_size, seq_len, d_model)`.
    return x
```

Let us focus on the two forms of Attention

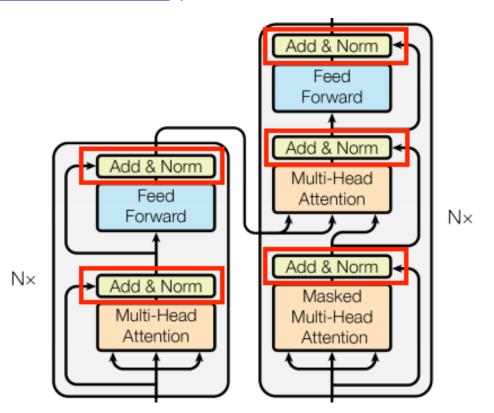
- context is the Encoder output
- x is the Decoder input

The Causal Self-Attention uses query x (at each position) to attend to entire sequence x.

• the attention is *causual*: for each position, future positions *may not* be attended to

The Cross-Attention uses query x (at each position) to attend to Encoder output context

<u>Add and Normalize</u> (<u>https://www.tensorflow.org/text/tutorials/transformer#add_and_normalize</u>)



Review: Layer Normalization

- The variance of outputs tends to grow from layer to layer
- Large variance causes gradient updates to become unstable
- <u>Layer Normalization</u>
 (https://proceedings.neurips.cc/paper files/paper/2019/file/2f4fe03d77724a72170

 <u>Paper.pdf</u>) reduces the variance of the input distribution to unit variance

SUBTLETY

The output of Attention layers (both Self Attention and Cross Attention) are feed into an Add & Norm block.

In what seems to be a "coding convenience"

- the code creates a common base class `BaseAttention(for both Self Attention and Cross Attention
- which facilitates the processing of Attention output through an Add & Norm block.

This is much more subtle than "coding convenience"!

The initializer creates sub-components

- Attention
- Layer Normalization
- Add

```
class BaseAttention(tf.keras.layers.Layer):
    def __init__(self, **kwargs):
        super().__init__()
        self.mha = tf.keras.layers.MultiHeadAttention(**kwargs)
        self.layernorm = tf.keras.layers.LayerNormalization()
        self.add = tf.keras.layers.Add()
```

but doesn't actually perform the normalization or addition.

- there is no call method of the base class
- these are left to the child (Attention) classes

Before we examine the child classes, let's examine the **purpose** of the Add & Norm block.

The "obvious" purpose is to normalize the Attention outputs

- using a tf.keras.layers.LayerNormalization layer
- that is the Norm part of Add & Norm

It is easy to miss the role of the Add part.

Mechanically: the Add is uninteresting.

The Add part adds the block's two inputs (i.e, Attention input and Attention output)

- before Normalization
- In both the Self-Attention and Cross Attention children, the call method performs the Add and Norm via statements

```
x = self.add([x, attn_output])
x = self.layernorm(x)
```

• where x is the Attention input and attn_output is the Attention output.

But what is the **purpose** of adding Attention input and Attention output?

This creates a residual or skip connection

- on the forward pass, the input to Attention can "skip over" the Attention block
- more importantly: on the backward pass: the loss gradient can skip over the Attention block

Review: Residual connections (RNN_Residual_Networks.ipynb#Residual-connections:-a-gradient-highway)

- Gradients can vanish or explode as they traverse an increasing number of layers during back propagation
- A zero gradient causes the Gradient update step to leave weights unchanged
 - the model can't "learn"
- The skip connection prevents gradients from vanishing or exploding by allowing them to by-pass one or more layers in the backward pass

So Add & Norm is much more than "good coding"

• observing that Attention outputs are always fed into common blocks

It is also the mechanism by which the residual connections are implemented.

Attention

The Self Attention (the class is called GlobalSelfAttention) and Cross Attention blocks are both derived from BaseAttention

which we explained in the section on "Add and Norm".

The sub-components (including the class MultiHeadAttention that implements Attention) are created by the parent class.

The child classes mainly implement the call method

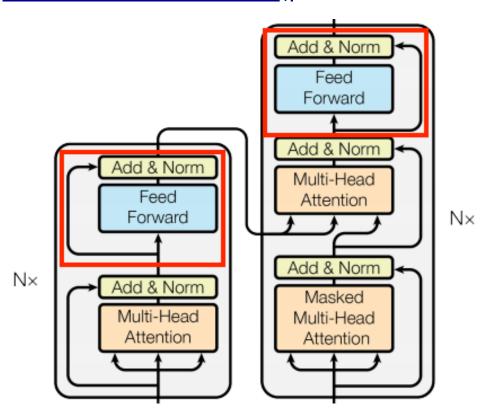
- that invokes the sub-components in sequence
- and implement the residual connection

For Self-Attention, the call is

```
class GlobalSelfAttention(BaseAttention):
    def call(self, x):
        attn_output = self.mha(
            query=x,
            value=x,
            key=x)
    x = self.add([x, attn_output])
    x = self.layernorm(x)
    return x
```

For Cross Attention, the call is

<u>Feed forward</u> (https://www.tensorflow.org/text/tutorials/transformer#the_f eed_forward_network)



The purpose of the Feed Forward block

- is to transform the Decoder Cross Attention output at each position into a "prediction"
 - of the next token (that is the Language Model objective

The typical Feed Forward network is two Dense layers

- the first has $d_{
 m ff}$ units
 - lacktriangledown creating $d_{
 m ff}$ synthetic features from the $d_{
 m model}$ features of the Attention output
- ullet the second has $d_{
 m model}$ units
 - lacktriangledown re-sizing the output to the standard $d_{
 m model}$ output size of all blocks in a Transformer through two Dense layers.

In the original paper

$$d_{
m ff} = 4*d_{
m model}$$

and this seems to have become a common choice.

Here is the code:

```
class FeedForward(tf.keras.layers.Layer):
    def __init__(self, d_model, dff, dropout_rate=0.1):
        super().__init__()
        self.seq = tf.keras.Sequential([
            tf.keras.layers.Dense(dff, activation='relu'),
            tf.keras.layers.Dense(d_model),
            tf.keras.layers.Dropout(dropout_rate)
        ])
        self.add = tf.keras.layers.Add()
        self.layer_norm = tf.keras.layers.LayerNormalization()

def call(self, x):
        x = self.add([x, self.seq(x)])
        x = self.layer_norm(x)
        return x
```

SUBTLETY

The Feed Forward output is passed to an Add & Norm block

- which has two inputs
 - Feed Forward output and Feed Forward input
 - the Feed Forward input is a residual connection
- similar to the residual connection we saw in the "Add and Normalize" section.

The residual connection is implemented in the call via the statements

```
x = self.add([x, self.seq(x)])
x = self.layer_norm(x)
```

where

- x is the input to the Feed Forward block
- self.seq(x) is the output of the Feed Forward block
 - the input passed through the two Denselayers, implemented as a Sequential model

<u>Training</u> (<u>https://www.tensorflow.org/text/tutorials/transformer#training</u>)

Teacher forcing

SUBTLETY

A Generative task (like the LLM objective) is exhibits Autoregressive behavior

• the Decoder output $\hat{\mathbf{y}}_{(t-1)}$ at position (t-1) is fed back as input for position t.

In the Transformer, the position (t-1) output is appended to all previous outputs.

Thus, at inference time: the input for position t is $\hat{\mathbf{y}}_{([1:t-1])}$

But, this **exact** behavior is not conducive to learning.

- Suppose $\hat{\mathbf{y}}_{(t-1)}$ is incorrect and not equal to correct label $\mathbf{y}_{(t-1)}$
- ullet this error cascades into the prediction of all subsequent positions $\hat{\mathbf{y}}_{([t:])}$

So, during ${f training}$ time: the input for position t is ${f y}_{([1:t-1])}$

- the *correct* sequence
- rather than the *predicted* sequence

This is called *Teacher Forcing* at training time

• but not at inference time

It's very easy to not notice Teacher Forcing when it occurs because it is subtle.

Can you see where it occurs?

It is in the *construction* of the Training examples

- ullet the input for position t are the features of example t: $\mathbf{y}_{([1:t-1])}$
 - *not* the Autoregressive constructed $\hat{\mathbf{y}}_{([t:])}$

During training, each example trains for one "step"

- so we don't see the effect of $\hat{\mathbf{y}}_{(t-1)}$ being fed back to the input for the next step t

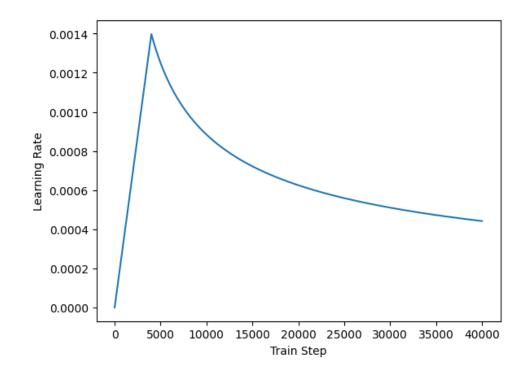
Custom Learning Rate Schedule

A custom learning rate schedule (subclassed from tf.keras.optimizers.schedules.LearningRateSchedule) is created

ullet varies learning rate lpha of Gradient update by epoch

$$\mathbf{W}_{(ext{epoch}+1)} = \mathbf{W}_{(ext{epoch})} - lpha * rac{\partial \mathcal{L}_{(ext{epoch})}}{\partial \mathbf{W}_{(ext{epoch})}}$$

- lacktriangle a warm-up period where lpha increases
- lacktriangle a post-warm-up period where lpha decays



<u>Loss and metrics</u> (<u>https://www.tensorflow.org/text/tutorials/transformer#set_up_the_loss_a_nd_metrics</u>)

Since the targets are Categorical values, Cross Entropy is used as a loss.

But: the target is a sequence with *padding*

- the padding should not figure into the Loss
- so the loss is "masked" whenever the target label is a padding token (0)

Similarly the Accuracy metric is modified so that padding characters don't participate in the calculation.

```
def masked loss(label, pred):
  mask = label != 0
  loss object = tf.keras.losses.SparseCategoricalCrossentropy(
   from logits=True, reduction='none')
  loss = loss object(label, pred)
 mask = tf.cast(mask, dtype=loss.dtype)
  loss *= mask
  loss = tf.reduce_sum(loss)/tf.reduce_sum(mask)
  return loss
def masked_accuracy(label, pred):
  pred = tf.argmax(pred, axis=2)
  label = tf.cast(label, pred.dtype)
 match = label == pred
 mask = label != 0
```

<u>Second example: Mini-GPT</u> (<u>https://keras.io/examples/generative/text_generation_with_miniature_gpt/)</u>

We will examine a notebook that builds a miniature version of GPT: <u>tutorial view</u> (<u>https://keras.io/examples/generative/text_generation_with_miniature_gpt/)</u>

 Colab notebook (https://colab.research.google.com/github/keras-team/kerasio/blob/master/examples/generative/ipynb/text_generation_with_miniature_gpt.ipy

We first see a definition of the constants:

```
vocab_size = 20000 # Only consider the top 20k words
maxlen = 80 # Max sequence size
embed_dim = 256 # Embedding size for each token
num_heads = 2 # Number of attention heads
feed_forward_dim = 256 # Hidden layer size in feed forward network inside tran
sformer
```

Relating the variable names to our notation

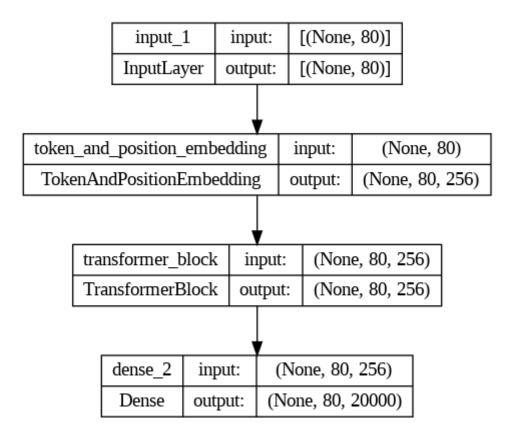
Notation	variable	value	
$d_{ m model}$	embed_dim	256	
T	max_len	80	
$n_{ m heads}$	num_heads	2	
	vocab_size	20,000	

And the Decoder model:

```
def create_model():
    inputs = layers.Input(shape=(maxlen,), dtype=tf.int32)
    embedding_layer = TokenAndPositionEmbedding(maxlen, vocab_size, embed_dim)
    x = embedding_layer(inputs)
    transformer_block = TransformerBlock(embed_dim, num_heads, feed_forward_di

m)
    x = transformer_block(x)
    outputs = layers.Dense(vocab_size)(x)
    model = keras.Model(inputs=inputs, outputs=[outputs, x])
    loss_fn = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)
    model.compile(
        "adam", loss=[loss_fn, None],
    ) # No loss and optimization based on word embeddings from transformer blo
ck
    return model
```

Here is the plot:



Examining each layer

- Input
 - lacksquare sequence (length T=80) of integers (index of a character within vocabulary) $\mathbf{y}_{(1:T)}$
- TokenAndPositionEmbedding
 - lacktriangledown maps sequence (length T=80) of integers (index of character)
 - lacktriangledown into sequence (length T=80) of $d_{
 m model}=256$ size representations
- TransformerBlock
 - lacktriangledown maps sequence (length T=80) into sequence of latents ${f h}_{(1:T)}$
 - o one latent per position in input

- Dense
 - Classifier layer
 - maps sequence of latents
 - to sequence of probability vectors
 - $^{\circ}\,$ each position is a probability vector of length <code>vocab_size</code> =20000
 - \circ position i: probability that output is element i of vocabulary
 - sum across positions in each vector is 100%

Loss function

The create_model method also defines the Loss Function

loss_fn = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)

as Cross Entropy, as is common for a Classifier

Notice that the SparseCategoricalCrossentropy takes a vector (of length vocab_size) of **logits** rather than **probabilities**.

TransformerBlock

Let's examine the <u>TransformerBlock (https://colab.research.google.com/github/kerasteam/keras-</u>

<u>io/blob/master/examples/generative/ipynb/text_generation_with_miniature_gpt.ipynb#scr_b)</u> in more detail

```
In [ ]:
             class TransformerBlock(layers.Layer):
                 def init (self, embed dim, num heads, ff dim, rate=0.1):
                     \overline{\text{super}}(\overline{)}. init ()
                     self.att = layers.MultiHeadAttention(num heads, embed dim)
                     self.ffn = keras.Sequential(
                          [layers.Dense(ff dim, activation="relu"), layers.Dense(embed di
        m),]
                     self.layernorm1 = layers.LayerNormalization(epsilon=1e-6)
                     self.layernorm2 = layers.LayerNormalization(epsilon=1e-6)
                     self.dropout1 = layers.Dropout(rate)
                     self.dropout2 = layers.Dropout(rate)
                 def call(self, inputs):
                     input shape = tf.shape(inputs)
                     batch size = input shape[0]
                     seq len = input shape[1]
                     causal mask = causal attention mask(batch size, seg len, seg len, t
         f.bool)
                     attention output = self.att(inputs, inputs, attention mask=causal ma
         sk)
                     attention output = self.dropout1(attention output)
                     out1 = self.layernorm1(inputs + attention output)
                     ffn output = self.ffn(out1)
                     ffn output = self.dropout2(ffn output)
                     return self.layernorm2(out1 + ffn output)
```

We can see that the TransformerBlock is implemented as a Layer (layers.Layer)

so it will translate its input into output via a call method

The class __init__ method defines the components of the Transformer

- stores them in instance variables:
 - Attention: self.att
 - Feed Forward Network FFN: self.ffn
 - Other: Layer Norms, Dropouts

The call method does the actual work

- ullet Masked self-attention to $\mathbf{y}_{(1:T)}$
 - Creates casual mask causal_mask to prevent peeking ahead at notyet-generated output
 - \circ seq_len is current length t of $\mathbf{y}_{1:t}$
 - Attention block self.att applied to causally-masked input attention_output = self.att(inputs, inputs, attention mask=causal mask)
- Dropout self.dropout1 and LayerNorm layernorm1 applied to attention output
- Result passed through Feed Forward Network self.ffn

TokenAndPositionEmbedding

Let's examine the <u>TokenAndPositionEmbedding</u> (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/generative/ipynb/text_generation_with_miniature_gpt.ipynb#scr_c

```
class TokenAndPositionEmbedding(layers.Layer):
    def __init__(self, maxlen, vocab_size, embed_dim):
        super().__init__()
        self.token_emb = layers.Embedding(input_dim=vocab_size, output_dim=embed_dim)

        self.pos_emb = layers.Embedding(input_dim=maxlen, output_dim=embed_dim)

def call(self, x):
    maxlen = tf.shape(x)[-1]
    positions = tf.range(start=0, limit=maxlen, delta=1)
    positions = self.pos_emb(positions)
    x = self.token_emb(x)
    return x + positions
```

We can see that it too is implemented as a Layer.

The call method

- translates the input sequence
 - each position in the sequence is an integer index within the vocabulary
- into a sequence of pairs
 - first element: token embedding

```
x = self.token_emb(x)
```

second element: position embedding

```
positions = tf.range(start=0, limit=maxlen, delta=1)
positions = self.pos_emb(positions)
```

As explained <u>in a prior module (Transformer_PositionalEmbedding.ipynb#Representing-the-combined-token-and-positional-encoding)</u>

- The output is not actually a sequence of *pairs*
 - it is a sequence of numbers
 - the token and positional emeddings are *added* not concatenated
 - o concatenation would double the length
 - \circ all layers in Transformer preserve output length equal input length = $d_{
 m model}$
- See the module's explanation as to why addition works

Dense (Feed Forward Network)

We can see that the Feed Forward Network are two Dense layers

We may have been expecting the final layer of TransformerBlock to be outputting a probability vector (over the Vocabulary)

- a vector of length vocab_size
 - lacktriangle position i is probability that output is element i of the Vocabulary
- using a softmax activation
 - to make sure sum (across the vocab_size elements of the vector) of probabilities is `00%

But we see that the output is

- a singleton (not a vector)
- ullet of size equal to embed_dim = $d_{
 m model}$

That is:

• the Dense component of the TransformerBlock is outputing the embedding of $\hat{\mathbf{y}}_{(t)}$ rather than a probability vector

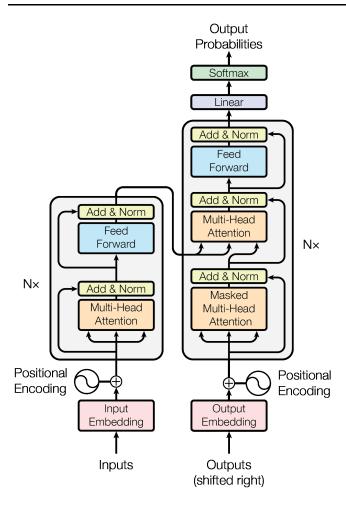
As we will see

- there is a layer in the Model *after* the TransformerBlock
- that produces the probability vector

Skip connections

Here is a more detailed view of the Transformer

Transformer (Encoder/Decoder)



In particular, please focus on the arrows into the "Add & Norm" layers.

These are *skip connections* that bypass the Attention layers.

• Residual Networks

Where is this reflected in the code?

It is a little subtle and easy to miss.

With the call method of the TransformerBlock please notice the statement

out1 = self.layernorm1(inputs + attention_output)

• inputs is the input to the Attention layer

attention_output = self.att(inputs, inputs, attention_mask=causal_mask)

So the addition

```
inputs + attention_output
```

is joining (via addition)

- the output of the Attetnion layer
- the input of the Attention layer

This is the skip connection!

Similar code appears

```
ffn_output = self.ffn(out1)
ffn_output = self.dropout2(ffn_output)
return self.layernorm2(out1 + ffn_output)
```

where

- the input to the FFN (i.e., out 1)
- is joined (via addition) to the output of the FFN (i.e., ffn_output)

```
out1 + ffn_output
```

Model

By examining the create_model function, we see that the output of the TransformerBlock

- is fed into a Dense layer
- which outputs a vector of length vocab_size (the correct length of a probability vector)
- and the output of this Dense layer is the output of the model
 - not the output of the TransformerBlock

```
outputs = layers.Dense(vocab_size)(x)
model = keras.Model(inputs=inputs, outputs=[outputs, x])
```

• Technically: the output vector is of *un-normalized logits* rather than probabilities

- the logit vector can be turned into a probability vector via a softmax

Thus, the Model outputs a vector of logits.

We can see how a token is sampled

- by converting the logit vector into a probability vector
- with the sample_from method of the TextGenerator callback def sample_from(self, logits):

```
logits, indices = tf.math.top_k(logits, k=self.k, sorted=True)
indices = np.asarray(indices).astype("int32")
preds = keras.activations.softmax(tf.expand_dims(logits, 0))[0]
preds = np.asarray(preds).astype("float32")
return np.random.choice(indices, p=preds)
```

Rather than outputting a probability vector

- which would require the user choosing one element from the vector (a word in the vocabulary)
- what is output is the embedding of the chosen word in the vocabulary

Since this output is compared against the correct label (i.e, $\mathbf{y}_{(t+1)}$ for position t)

• we should also see that the *labels* used are embeddings

Training

A <u>TextGenerator</u> (https://colab.research.google.com/github/keras-team/keras-io/blob/master/examples/generative/ipynb/text_generation_with_miniature_gpt.ipynb#scr <u>f</u>) call-back is used during training

- at the end every self.print every epochs
- a sample of $\hat{\mathbf{y}}_{(1:T)}$ will be drawn
- to illustrate what the model output would be up to that point in training

The heart of the call-back

```
while num_tokens_generated <= self.max_tokens:
    ...
    y, _ = self.model.predict(x)
    sample_token = self.sample_from(y[0][sample_index])
    ...</pre>
```

- ullet is a loop over positions t
- that extends a fixed input (prefix of text) start_tokens
- ullet to full length T
- ullet by sampling a token from the output for position t

This is useful

- to see whether our model is learning as epochs advance
- to confirm the shape and type of the model output is a vector of logits
 - the model output for position t: y, _ = self.model.predict(x)
 - is passed to sample_from
 - which samples from the probability distribution derived from the logits (model output)

```
In [2]: print("Done")
```

Done