Transformer: Intuition

We try to briefly explain what each the "moving parts" of the Encoder-Decoder style Transformer is doing.

At the highest level: we have the Encoder and the Decoder.

In the Encoder-Decoder architecture

- the Encoder completes before the Decoder starts

Encoder

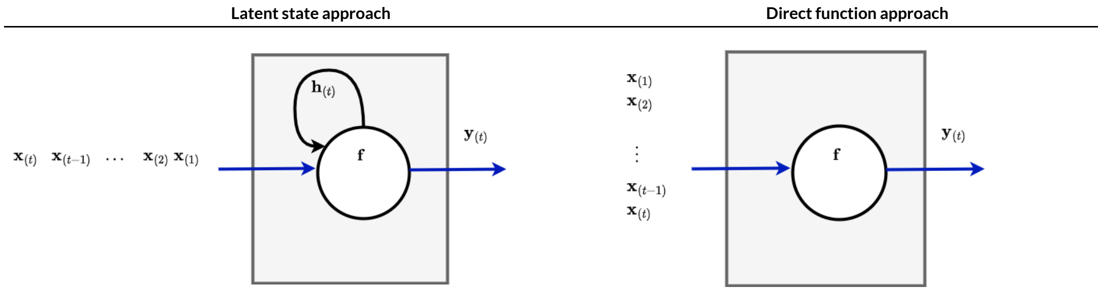
The role of the Encoder is

- to create a Context Sensitive Representation
$$\bar{\mathbf{h}}_{(1:\bar{T})}$$
- of each of the Encoder's input tokens
$$\mathbf{x}_{(1:\bar{T})}$$

It accomplishes this by the *direct function* approach

- unlike an RNN, it does not process each input token $\mathbf{x}_{(t)}$ sequentially
- it computes $\bar{\mathbf{h}}_{(t)}$ as a function of the entire input $\mathbf{x}_{(1:\bar{T})}$

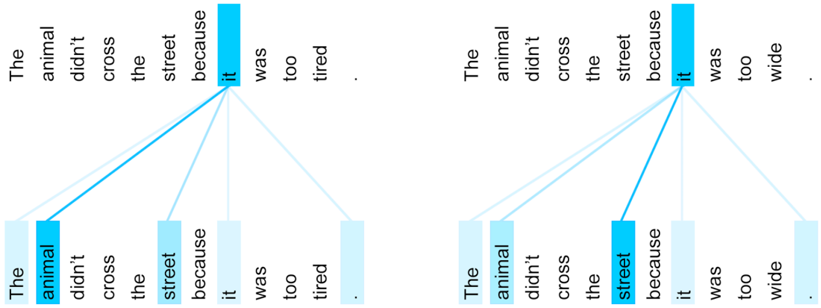
Encoder Self-Attention is used in the direct function.



By making the meaning dependent on the full context, we can disambiguate the meaning of the world "it"

Attention weights

Thickness of the blue lines indicate the strength of attention to other tokens



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Decoder

The Decoder works in *auto-regressive* mode

- predicts one output token at a time
- the current output $\hat{\mathbf{y}}_{(t)}$ token is appended to the input for the next position
    - so the input at time step t is
    $$\hat{\mathbf{y}}_{(1...t-1)}$$

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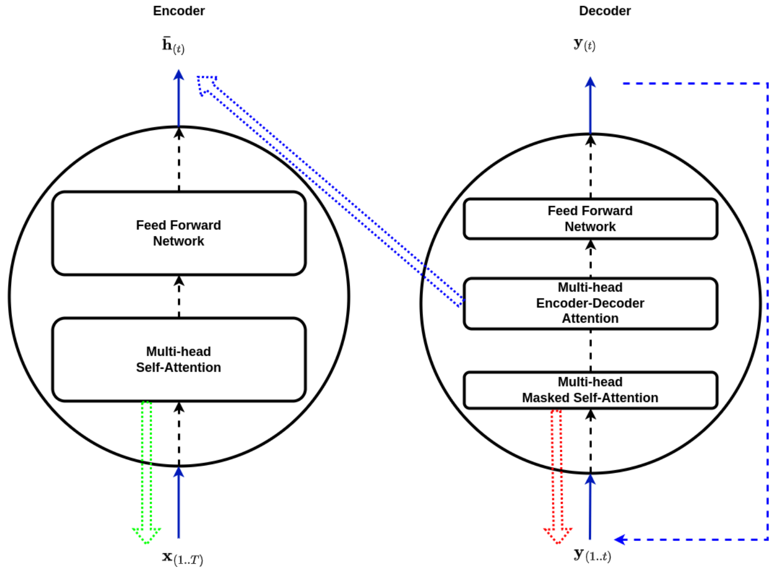
Encoder/Decoder transformer
Decoder: Cross-Attention, Auto-regressive mode



It has two inputs at step t

- the previously-generated output tokens t is
$$\hat{\mathbf{y}}_{(1\ldots t-1)}$$
- the Encoder output
$$\bar{\mathbf{h}}_{(1:\bar{T})}$$

Self-attention is used on $\hat{\mathbf{y}}_{(1\ldots t-1)}$

Cross-Attention is used on $\bar{\mathbf{h}}_{(1:\bar{T})}$

At step t, the Decoder

- uses Self-Attention on $\hat{\mathbf{y}}_{(1...t-1)}$
- to create a *query*
- that is used to attend to $\bar{\mathbf{h}}_{(1:\bar{T})}$

We can think of this use of Self-Attention

- as being a replacement for the "latent" state of an RNN
    - rather than using the latent state to record
        - what has already been done
        - what is the next step to perform
    - Self-Attention allows direct access to what has already been done: $\hat{\mathbf{y}}_{(1...t-1)}$

The query is used in Cross-Attention

- to attend to the Context Sensitive Representation of the input sequence $\mathbf{x}$

Whatever is returned by Cross-Attention

- is input into the Feed Forward Network (FFN)

Think of the FFN

- as a repository of "world knowledge" accumulated by processing the training data
- "facts"

The FFN produces an output

- which is processed by a Classifier (Linear layer)
- to produce a token in the vocabulary of tokens

That is

- if the vocabulary has $|V|$ tokens
- the Classifier produces a probability distribution vector $\mathbf{p}$ of length $|V|$)
    - such that $\mathbf{p}_j$ is the probability that the output token should be V_j

The exact mechanics of this multi-step process

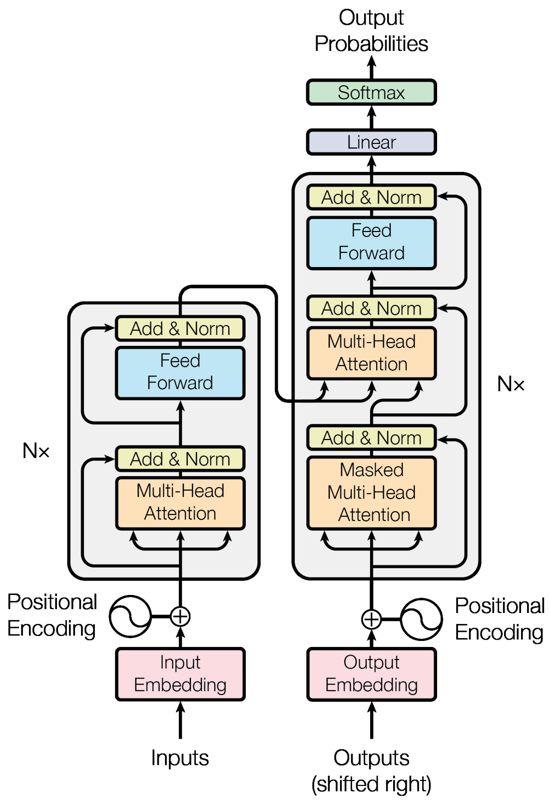
- are controlled by the weights
- that are learned during training

General

Here is the detailed architecture of the Encoder-Decoder Transformer.

We will review each of the pieces.

Transformer (Encoder/Decoder)



Each of the paths in the Transformer is a vector of length d_{model}

- sometimes just referred to as d

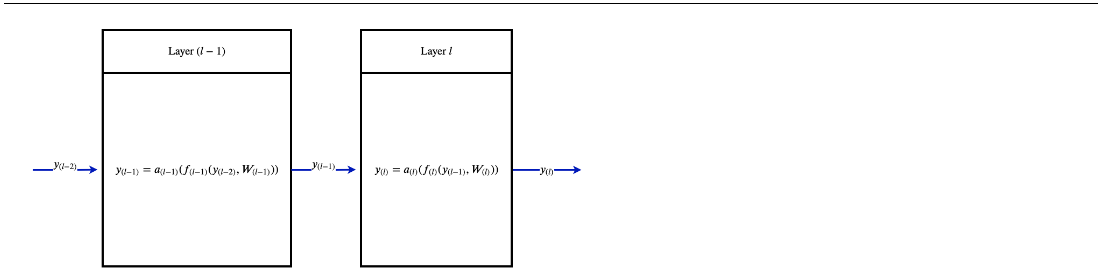
Having a common length simplifies the architecture

- can stack Transformer blocks (since input and output are same size)
- Self-Attention and Cross-Attention:
    - map a query of size d to an output of size d
- Needed for the Residual Connection (Add and Norm)
    - adding the input of Attention to the output of Attention
        - need to be same length

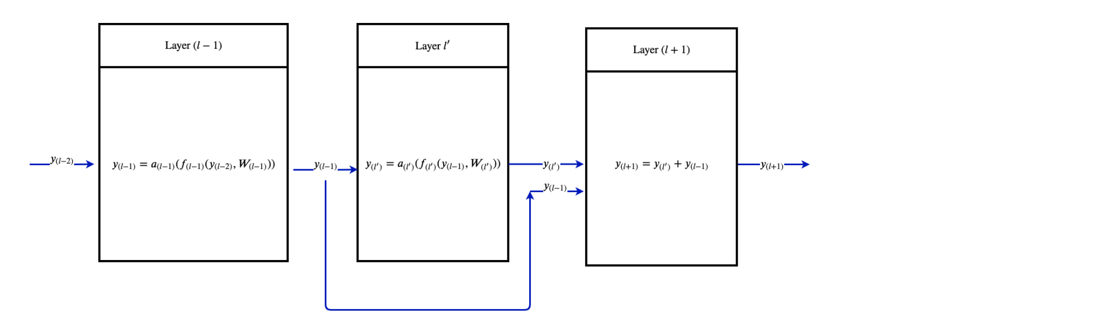
Residual connections

- [Residual connections from Intro course (RNN_Residual_Networks.ipynb)]()

Network, no Skip Connection



Residual Network with Skip Connection



Suppose we wanted the two networks to compute the same mapping from input $\mathbf{y}_{(l-1)}$ to output

$$\mathbf{y}_{(l+1)} = \mathbf{y}_{(l)}$$

Then

$$\begin{array}{lll}
\mathbf{y}_{(l+1)} & = & \mathbf{y}_{(l')} + \mathbf{y}_{(l-1)} & \text{definition of } \mathbf{y}_{(l+1)} \text{ in last layer of residual network} \\
\mathbf{y}_{(l)} & = & \mathbf{y}_{(l')} + \mathbf{y}_{(l-1)} & \text{requiring equality of outputs of the two networks } \mathbf{y} \\
\mathbf{y}_{(l')} & = & \mathbf{y}_{(l)} - \mathbf{y}_{(l-1)} & \text{re-arranging terms}
\end{array}$$

The intermediate layer l' we introduced in the Residual network computes

- the *residual*: of the original networks layer l output wrt to its' input: $(l-1)$ output

Embedding

Words (really: tokens) are *categorical* variables.

Categorical variables are usually encoded as long vectors via One Hot Encoding (OHE)

- very long: number of distinct elements in class
    - e.g., number of words in vocabulary
- *sparse*: only a single non-zero element in the vector

Biggest issue with OHE:

- the similarity (e.g., dot product) of two related words (e.g., "cat", "cats") is zero !
    - same as for two unrelated words (e.g., "cat", "car")

word	**rep(word)**	**Similarity to "dog"**
dog	[1,0,0,0]	rep(word) · rep(dog) = 1
dogs	[0,1,0,0]	rep(word) · rep(dog) = 0
cat	[0,0,1,0]	rep(word) · rep(dog) = 0
apple	[0,0,0,1]	rep(word) · rep(dog) = 0

An *Embedding* is a a *short* and *dense* vector representation of words (tokens).

In addition to being shorter (and dense: many non-zero elements possible) their construction results in

- the similarity of embeddings for two related words being *non-zero*

This makes Embeddings much more valuable for NLP.

$\boldsymbol{w}$	$\mathbf{v}_{\boldsymbol{w}}$
cat	[.7, .5, .01]
cats	[.7, .5, .95]
dog	[.7, .2, .01]
dogs	[.7, .2, .95]
apple	[.1, .4, .01]
apples	[.1, .4, .95]

The *Embedding Layer* converts the OHE representation to an Embedding.

See the module from the Intro course (NLP_Embeddings.ipynb) for details.

Positional Encoding

The Transformer input is a *sequence*

- there is a total ordering between elements based on absolute position

The Transformer needs to be able to discern

- at least: the *relative* ordering of two elements in different positions in the sequence

The *Positional Encoding* layer

- adds a vector that encodes position
- to the Embedding
- such that the Transformer has a representation with both meaning and positions

This is much more involved than simply using an integer to encode the position.

The fundamental operation of a Neural Network is matrix multiplication

- the positional encoding needs to be preserved as it traverses the layers

The details are not trivial.

See the module on Positional Embeddings (Transformer_PositionalEmbedding.ipynb) if you are interested.

Layer Normalization (part of Add and Norm)

We show in a [module (Training_Neural_Networks_Scaling_and_Initialization.ipynb#Importance-of-unit-variance-across-features)](Training_Neural_Networks_Scaling_and_Initialization.ipynb#Importance-of-unit-variance-across-features) from the Intro course that

- The variance of the *pre-activation distribution* of features grows with the depth of the network.

That is

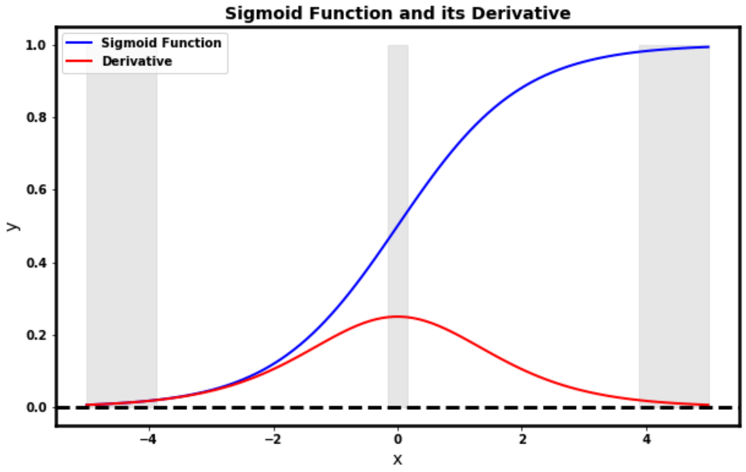
- even if we standardize all the input (Layer 0) features
- the variance of features in layers $l > 0$ tends to grow

As the variance of the pre-activation gets larger

- we are more likely to be in one of the extremes of the domain of the Activation function
- where derivatives are often near-zero
- and thus: weights don't get updated during Gradient Descent

Hence, we wind up in an unfavorable region of the Activation function.

Sigmoid and it derivative
Shaded regions indicated second derivative near 0



A [Normalization Layer (Training_Neural_Networks_Scaling_and_Initialization.ipynb#Batch-Normalization-Layer)](Training_Neural_Networks_Scaling_and_Initialization.ipynb#Batch-Normalization-Layer)

- re-normalizes its input features
- to mean 0 and unit variance

Feed Forward Network (FFN)

Maps the output of the Decoder-Encoder Attention into the "next output token".

- actually: it is still an embedding of the next token, rather than the true next token
    - that way: it can be appended to the already-generated output to become the Decoder input for next position

This acts as a Classifier

- mapping the input
- to a vector of logits
    - one element per possible element of the Output Vocabulary

There is some evidence that

- the parameters of the FFN are where "world knowledge" is stored
    - every "fact" learned during training

Linear

This layer is append *only* to the final block in the stacked Transformer blocks.

It acts as a typical Classifier

- "classifies" the final block's output of length d
- returning a vector
    - whose length is equal to number of elements of the Vocabulary
    - each element is a logit
        - to be converted into probability distribution over elements of the Vocabulary

Softmax

Converts the logit for each possible element of the Vocabulary

- into Probability that the element is the next Decoder Output

In [2]:

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print("Done")
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Done
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