Quick Intro: Attention Heads and Transformer Layers

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Outline

- Basic word prediction task and motivating the attention strategy
- A basic Attention Head network
- Transformers
- Exercise: Working with BERT pretrained transformer model

Dependences of Language

Consider this sequence:

The Law will never be perfect, but it’s application should be just - this is what we are missing, in my opinion <End of Sequence>

What does ‘it’ refer to that can have an ‘application’?

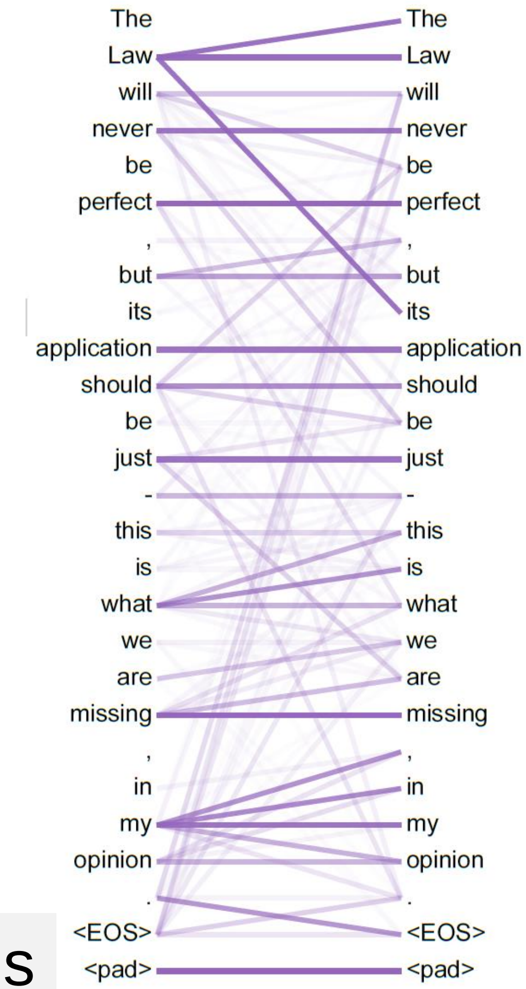
Dependences of Language

Consider this sequence:

The Law will never be perfect, but it's application should be just - this is what we are missing, in my opinion <End of Sequence>

What does 'it' refer to that can have an 'application'?

e.g 'it' refers back to 'Law', which is part of 'the Law' noun phrase, which is the entity that will 'never be perfect', and so on …



many dependencies and interactions

A toy problem to get some intuition

- Let's use the following list of 5 tokens:

  <start>, the, man, chicken, ordered

- Let's use this sequence of 6 tokens as our only:

  <start> the man ordered the chicken

- If we use token ids 1 to 5 it is the sequence of 6 numbers [1,2,3,5,2,4]

- **Now let's try to predict the next word by 'attention' idea**

The toy task: predict next word

The data: 5 tokens (V=5),

1 sequence (length=T=6):   <Start> the man ordered the chicken

A basic solution is bigram matrix

eg a sequence of tokens (rows) and current word predictions (cols)

X= Sequence-to-Word is TxV

Pos	Word	<strt>	The	Man	Chikn	Order.
0	<start>		1.0			
1	The			0.5	0.5	
2	Man					1.0
3	Orde.r		1.0			
4	The			0.5	0.5	
5	Chick.	1.0				

The toy task: predict next word

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Challenge, can we learn predictions (→) that depend on context of other tokens and/or position

After <Start> the → man = 1.0

After ‘Ordered’ the → chicken = 1.0

Pos	Word	<strt>	The	Man	Chikn	Order.
0	<start>		1.0			
1	The			0.5	0.5	
2	Man					1.0
3	Orde.r		1.0			
4	The			0.5	0.5	
5	Chick.	1.0				

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The attention idea

Let’s get all tokens to ‘pass information’ about dependencies

E.G. for *X a TxV* matrix, we want *W a TxT* matrix – aka ‘attention’ weights - so that *W*X=TxV* has contextual predictive information

W dependencies is TxT **X= Sequence-to-Word is TxV**

$$\begin{pmatrix} w_{11} & \cdots & w_{1T} \\ \vdots & \vdots & \vdots \\ w_{T1} & \cdots & w_{TT} \end{pmatrix} * \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0.5 & 0 \\ 1.0 & 0 & 0 & 0 & 0 \end{pmatrix} \to\to \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

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W will be learned and should depend on transformations of X

Making predictions causal

(ie only depends on previous tokens)

First build a TxT mask so that sequence position t only uses columns 1:t

$$Mask = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$

Then, multiply it by *W_dep* matrix

Now multiply masked dependency elementwise to W

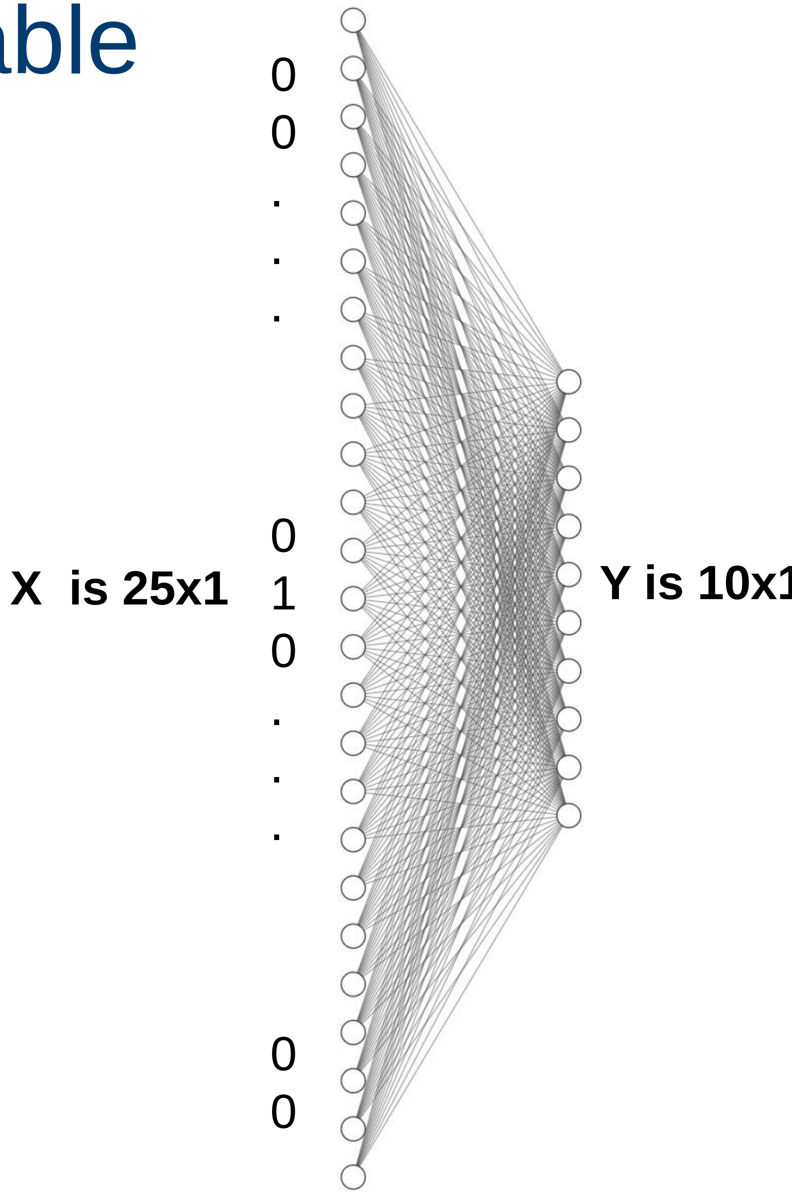
$$W_{dep} \odot Mask = \begin{pmatrix} w_{11} & 0 & \cdots & \cdots & 0 \\ w_{21} & w_{22} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ w_{T1} & w_{T2} & w_{T3} & \cdots & w_{TT} \end{pmatrix}$$

Finally, apply Softmax to each row to make it like probability weights

Transformation as Embedding Layer/Table

Let *X* be given as a 'one-hot vector input' – where one of the 25 input nodes is 1, the rest are 0.

Use linear activation so that $Y = W * X$



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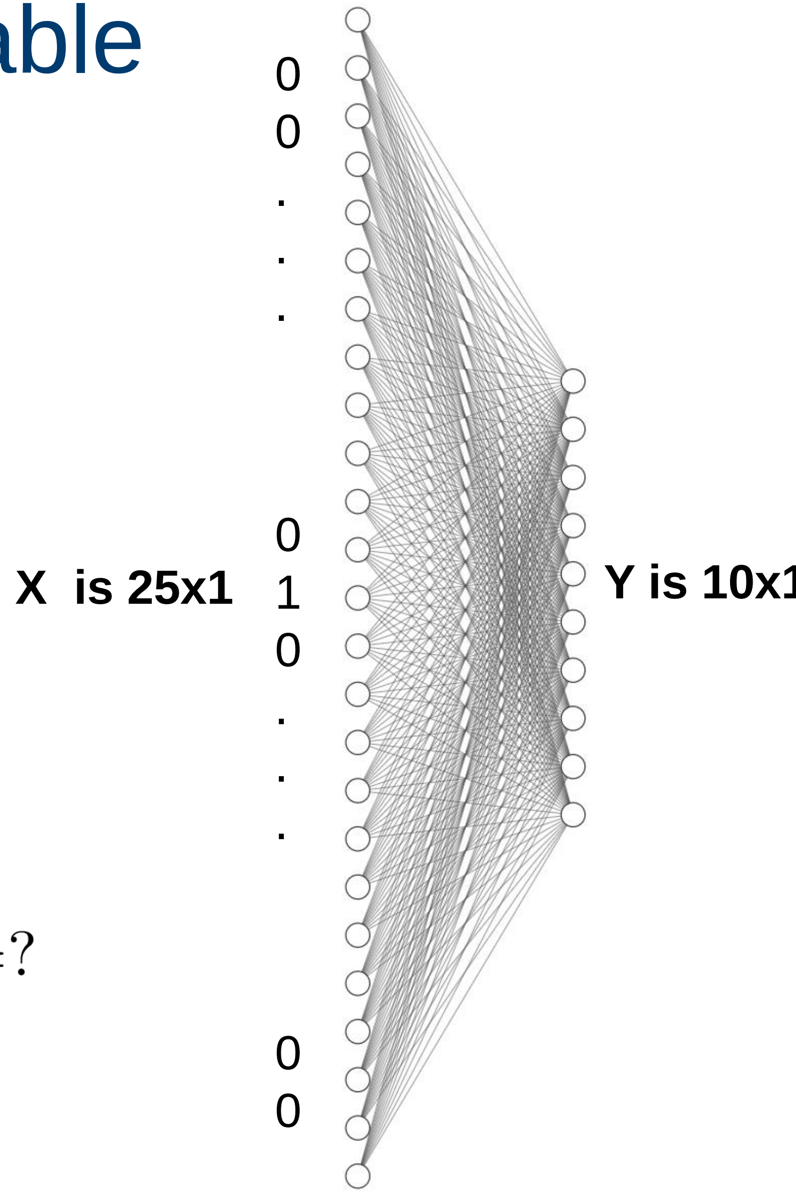
If j-th node is 1, then for *W* a 10x25 matrix

$$Y = W * X$$

$$= \begin{pmatrix} | & | & \cdot & | & \cdot & \cdot \\ w1 & w2 & \cdot & w_j & \cdot & \cdot \\ | & | & \cdot & | & \cdot & \cdot \end{pmatrix} * \begin{pmatrix} 0 \\ 0 \\ . \\ 1 \\ . \\ . \end{pmatrix} = ?$$



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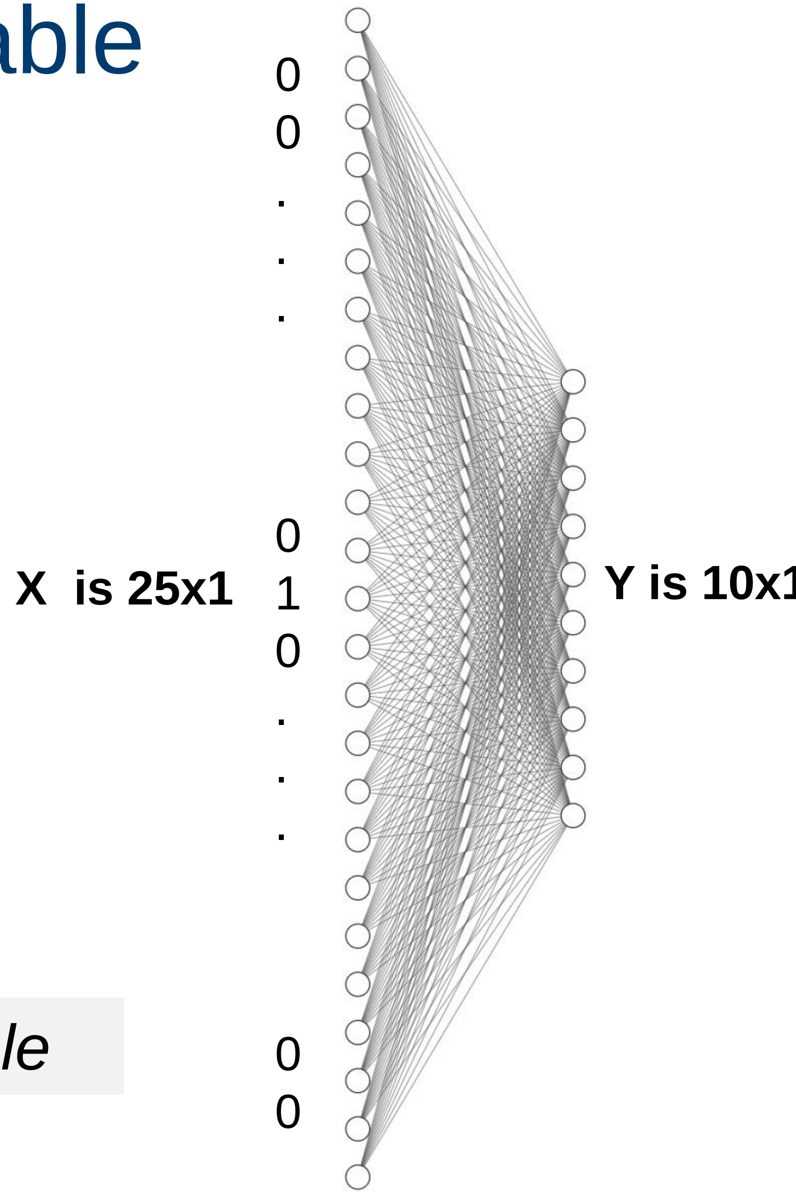
$$Y = W * X = W_j = \begin{pmatrix} | \\ w_j \\ | \end{pmatrix}$$

So just let X be sequence of token ids and treat W like a table



An Attention Head construction

1. Let X = sequence of token ids

For embedding dimension E, map: $\underset{T\times 1}{\mathrm{X}} \rightarrow \underset{T\times E}{Xemb}$

For positions 1...T map: $\underset{T\times 1}{\mathrm{P}} \rightarrow \underset{T\times E}{Xpos}$

Take as new input: $X = Xemb + Xpos$

2. For dimension H, get Q,K,V matrices: $\underset{T\times E}{\mathrm{X}} \rightarrow \underset{T\times H}{Query}$ $\underset{T\times E}{\mathrm{X}} \rightarrow \underset{T\times H}{Key}$ $\underset{T\times E}{\mathrm{X}} \rightarrow \underset{T\times H}{Value}$

3. Get Attention Weights and Output: $\underset{T\times H}{\mathrm{Q}} * \underset{H\times T}{\mathrm{K}'} \rightarrow \underset{T\times T}{\mathrm{W}_{\mathrm{dep}}}$

$$Output = softmax(W_{dep} \odot Mask) * V$$

All mappings are linear transformations

An Attention Head code

Hyperparameters:

E is for embedding dimension,

H is for “head size” (dimension) of transformations (we could let E = H)

11 Layers/Functions

```
#Now build model to learn transformation for Q,K,V matrices

Xsequence      = tf.keras.layers.Input(shape=(T,V)) #the batch size is left unspecified
Pos_Input      = tf.keras.layers.Input(shape=(T)) #just the t=1...T integer
Pos_Embed      = tf.keras.layers.Embedding(T,V, input_length=T,name='PosEmbed')(Pos_Input) #input wi
Xinputs        = tf.keras.layers.Add()([Xsequence, Pos_Embed])

#now feed to Q,K,V transformations
Qmat        = tf.keras.layers.Dense(H,activation='linear',use_bias=False,name='Qmat')(Xinputs) #so f
Kmat        = tf.keras.layers.Dense(H,activation='linear',use_bias=False,name='Kmat')(Xinputs)
Vmat        = tf.keras.layers.Dense(H,activation='linear',use_bias=False,name='Vmat')(Xinputs)

#now apply QtoK take softmax, scale it , apply to V
QK            = tf.keras.layers.Dot(axes=(2))([Qmat,Kmat])  #it will treat each Batch item separately
QKscaled      = tf.keras.layers.Lambda(lambda x: x * scale_constant)(QK)    #for each x in QK mult by
Attn_Wts       = tf.keras.layers.Softmax(axis=2,name='AttnWts')(QKscaled, mask=Msk)        #apply mas
Vout        = tf.keras.layers.Dot(axes=1,name='Voutput')([Attn_Wts,Vmat])

my_attn_model    = tf.keras.Model(inputs = [Xsequence,Pos_Input], outputs=Vout)
```

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Also a scaling by H

$$\text{softmax}(\underbrace{\frac{QK^T}{\sqrt{d_k}}})V$$

An example of attention head with a toy task:
(in the CIML23_toytask_attention notebook)

CIML23_toytask_attentionhe×

Markdown

Python 3 (ipyke

Let's use the following list of words (and a special token): , the, man, chicken, ordered,woman, beef 7 words,so V=7, and token ids are 1 to 7

This our corpus:
man ordered the chicken

woman ordered the beef

The corpus will be translated to 2 sequences of token ids as input.

Exercise Instructions: Let's examine the Attention Wt matrix to see how dependencies might be encoded (look for '<<<-----' markers)

Output TxV predictions:

Notice that the→ [chicken or beef] predictions change

```
1/1 [==============================] - 0s 106ms/step

 This is the output predictions use Head size 20
         <ST>    the    man   chkn  ordrd  woman   beef
0 <ST>  0.596  0.037  0.988  0.202  0.193  0.988  0.077
1 man   0.062  0.579  0.575  0.243  0.996  0.184  0.802
2 ordrd 0.092  0.991  0.122  0.612  0.319  0.050  0.403
3 the   0.225  0.705  0.016  0.996  0.008  0.018  0.837
4 chkn  0.994  0.103  0.365  0.679  0.104  0.634  0.333

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2 ordrd 0.129  0.994  0.049  0.626  0.153  0.034  0.511
3 the   0.028  0.686  0.163  0.727  0.786  0.034  0.992
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```

TxT Attn Wts:

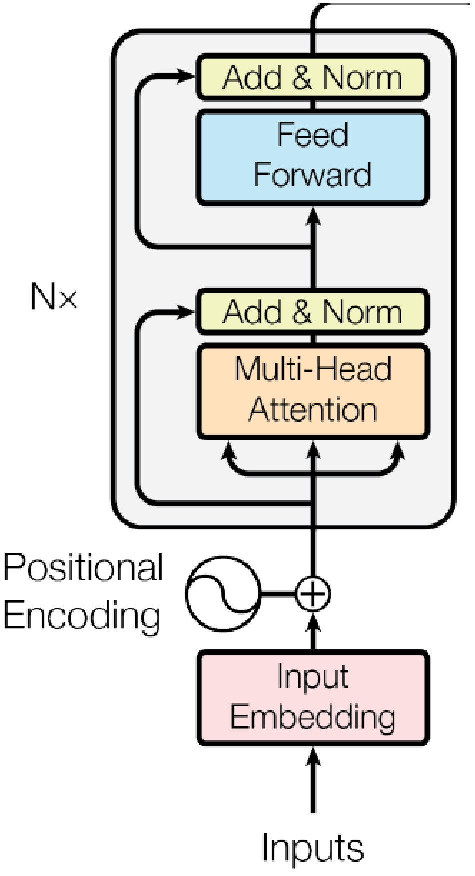
Notice that the ← wts are from [ordered or man]

```
for i-th input: 0   These are the output at layer  AttnWts
         0 <ST>  1 man   2 ordrd  3 the  4 chkn
0 <ST>    1.000  0.000    0.000  0.000   0.000
1 man     0.093  0.907    0.000  0.000   0.000
2 ordrd   0.064  0.561    0.375  0.000   0.000
3 the     0.003  0.213    0.759  0.025   0.000
4 chkn    0.258  0.003    0.160  0.523   0.056
The head size H was:  20
for i-th input: 1   These are the output at layer  AttnWts
         0 <ST>  1 woman  2 ordrd  3 the  4 beef
0 <ST>    1.000    0.000    0.000  0.000   0.000
1 woman   0.079    0.921    0.000  0.000   0.000
2 ordrd   0.091    0.374    0.535  0.000   0.000
3 the     0.001    0.769    0.223  0.007   0.000
4 beef    0.252    0.001    0.162  0.526   0.059
The head size H was:  20
```

Finally, a transformer

Include skip-add connections

Include Layer Normalization or DropOut layers



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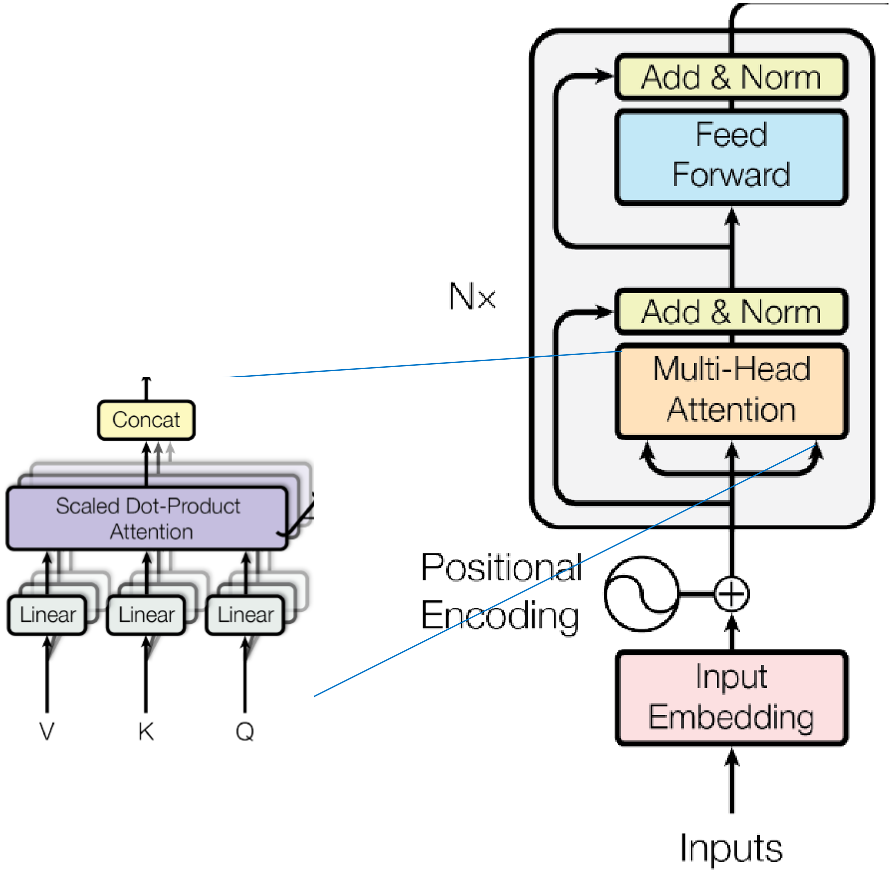
Multi-Head – for N heads produce *Tx(H/N)* each



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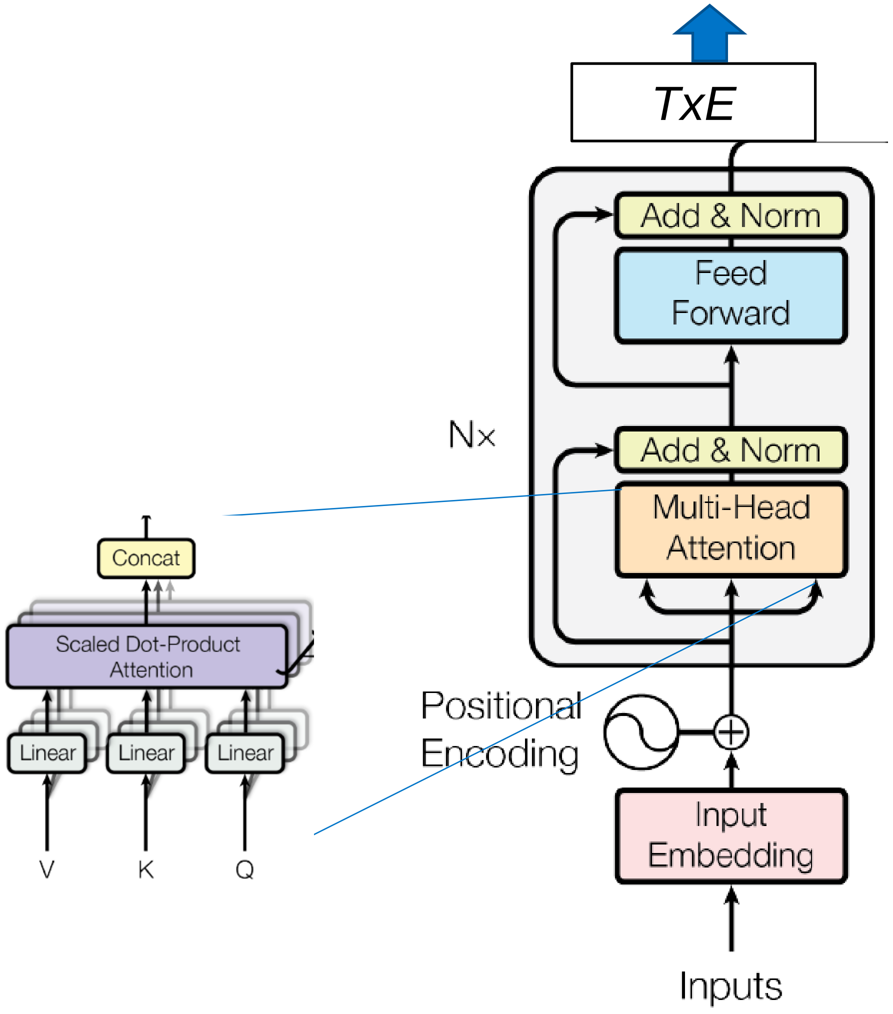
Add MLP layers on top –

output another *TxE* matrix stackable!



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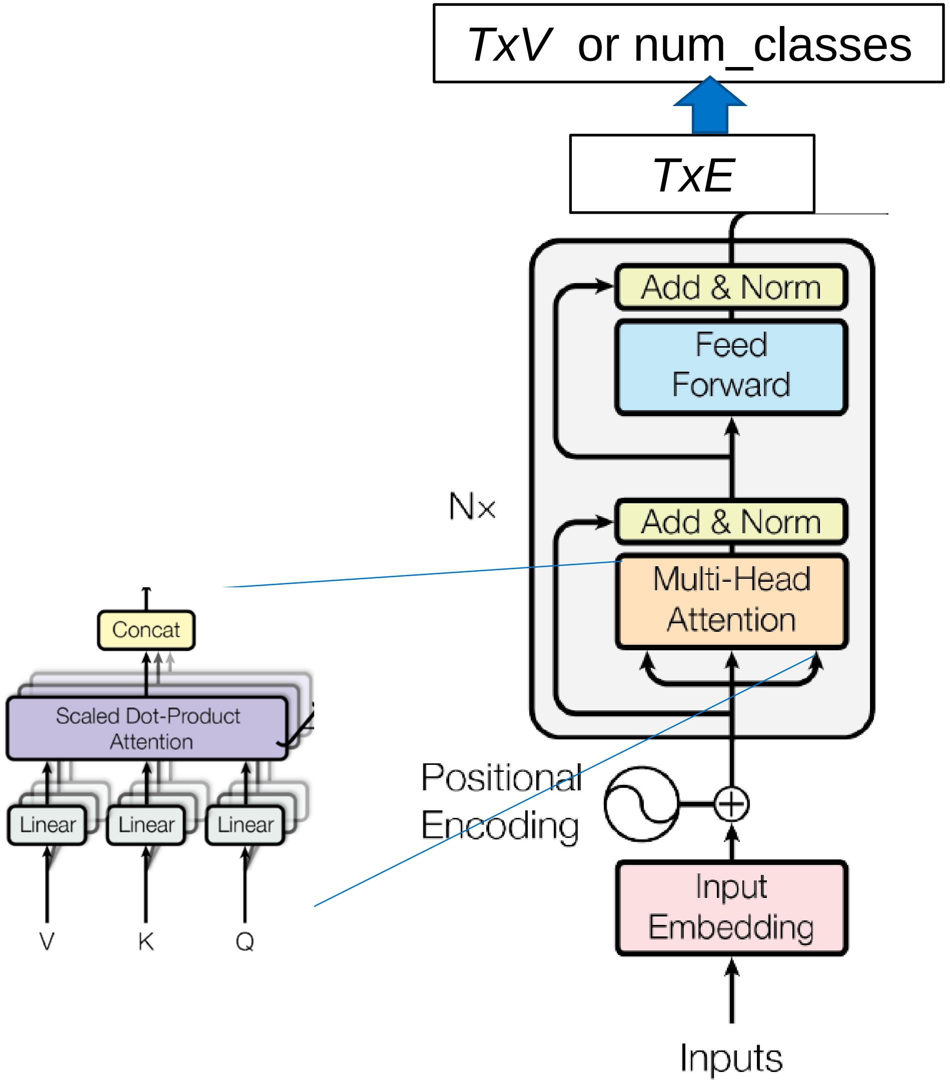
or output final probabilities



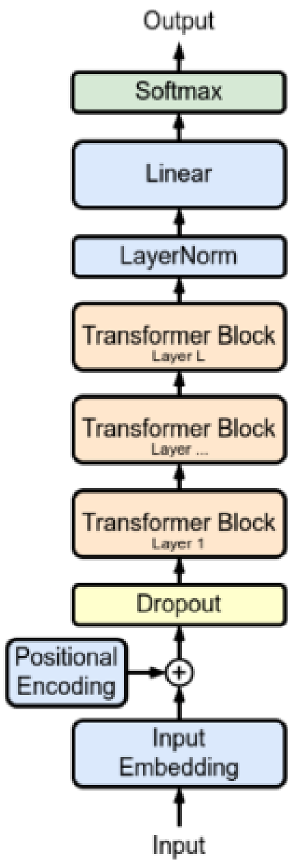
2 kinds of training strategies

GPT – predict next word only look back at prior context (which could be a whole document)

Put mask on attention weights so that predictions only depend on previous tokens

BERT – ***No attention mask*** so all token dependencies can influence all other tokens predictions

Special tokens help create a variety of tasks



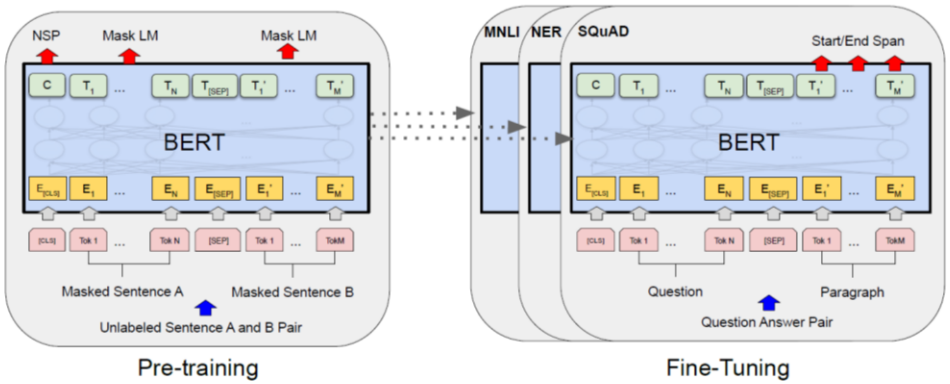
BERT (Bidirectional Encoder Representations from Transformers)

Goal: Train a model to develop general token-level AND sentence-level encoding

1 Pretrain on:

- fill-in-the-blank

- binary classification if 2 sentences go together



Devlin, etal, 2019

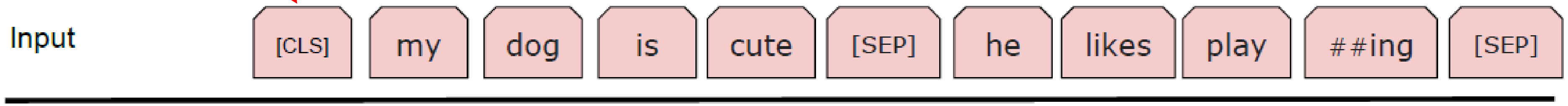
2 Fine tune on variety of tasks

BERT Input: 2 sentences

[CLS]
is'dummy' token and always present

[SEP] marks separation between sentences or sequences

[PAD] tokens help fill out sequence to T items



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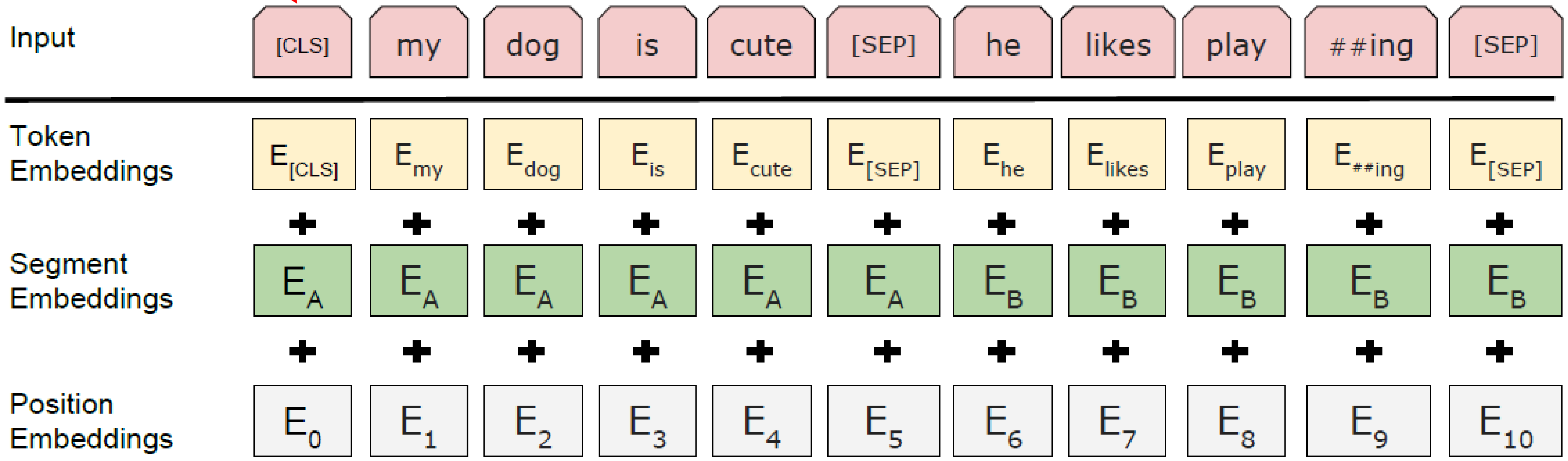


Add a TxE matrix for 'A" vs 'B' sentence

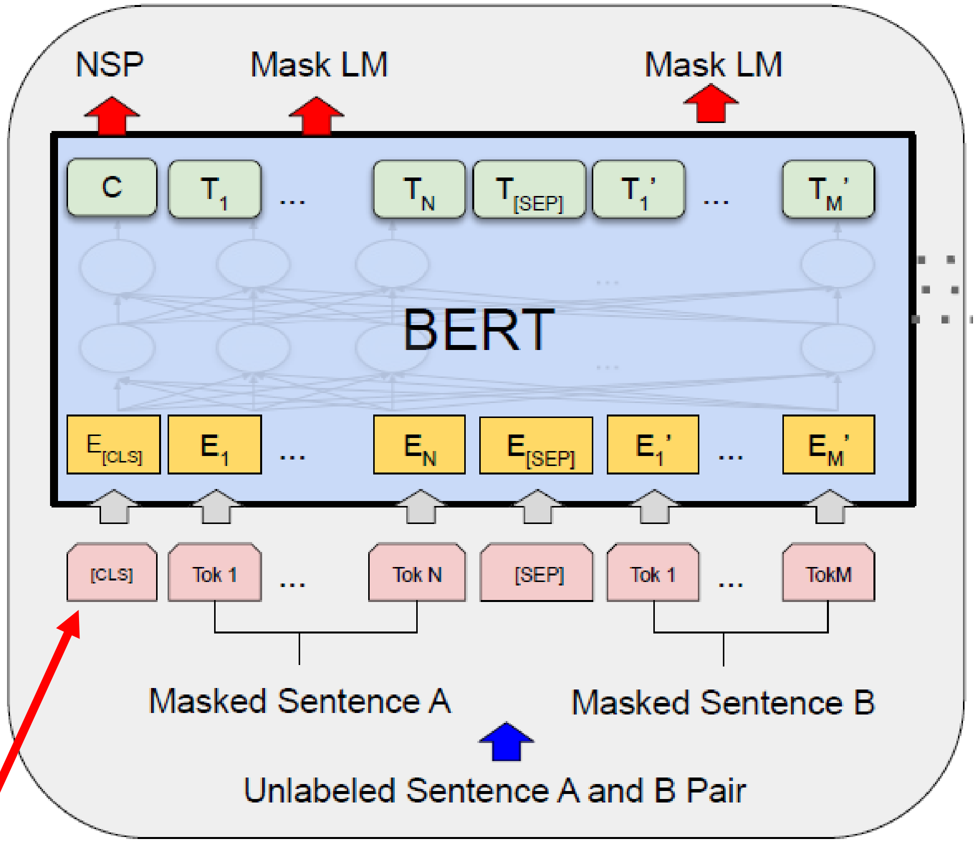
BERT –

Last layer *TxV* output

Transformer Layers

Embeddings

T Input tokens



Pre-training

[CLS] is'dummy' token and always present

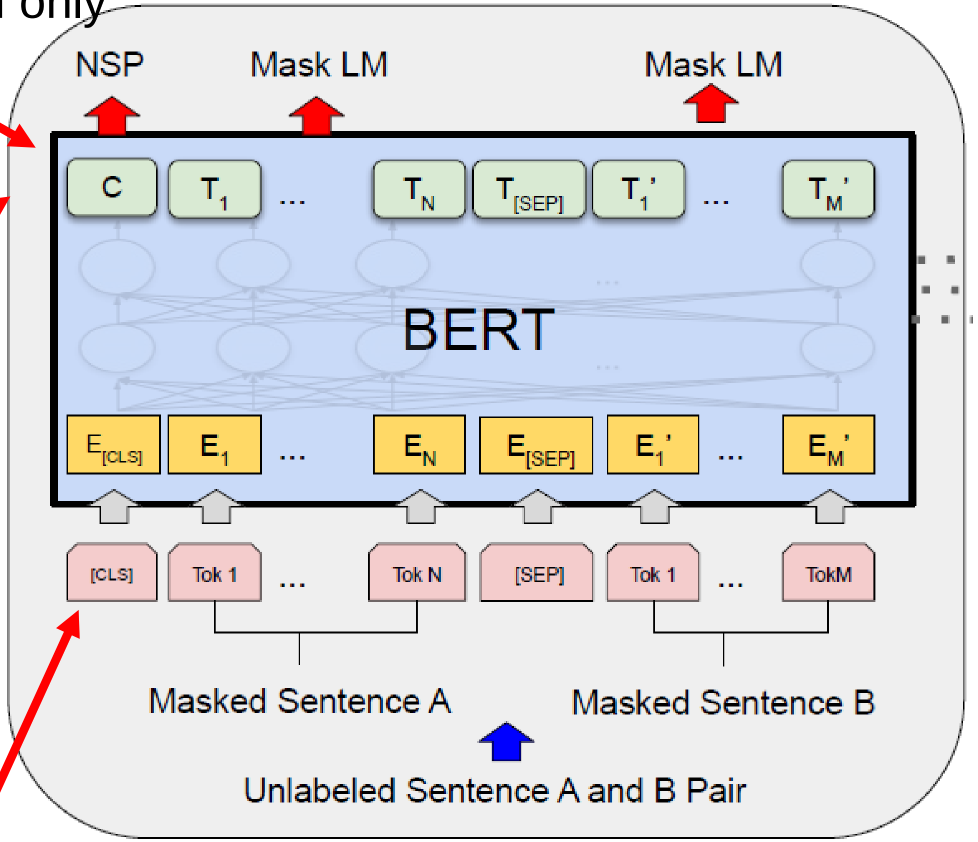
Devlin, etal, 2019

BERT –

For classification over paired sentences or any text, train C row vector (in the last layer *TxV* output matrix)

"NSP": classify if next sentence follows first sentence

Train a classification task on this [CLS] token prediction only



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KerasNLP

- KerasNLP is an extension to Keras

- KerasNLP has several pre-trained LLMs (large language models). Each model comes with related modules, for example:

  - GPT2Backbone the model without task specific output layers
  - GPT2CausalLM the model with output predictions
  - GPT2CausalLMPreprocessor the preprocessor that feeds model.fit

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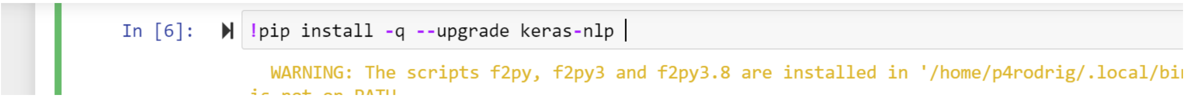
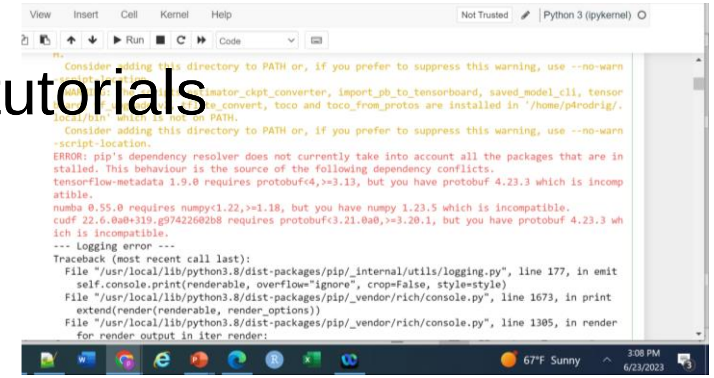
We will use pre-trained BERT and compare different BERT versions

Keras NLP package is not in the tensorflow container, so we can do:

1. Rebuild Container - check
2. Set up conda environment
3. Run ‘pip install’ commands



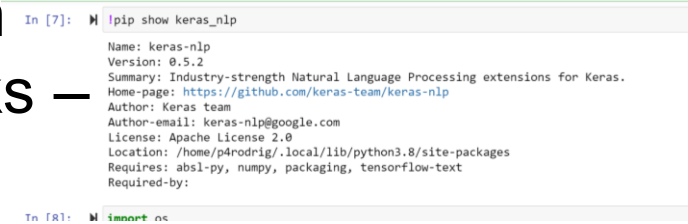
Option 3 is quick and a bit dirtier, but often useful and part of tutorials



On Expanse you might get warnings or logging errors.

But it should show the package as installed

Note, ‘pip install’ will put packages in .local directory which is on PythonPath. So there’s a potential to clash with other notebooks – you may have move/manage your .local directories

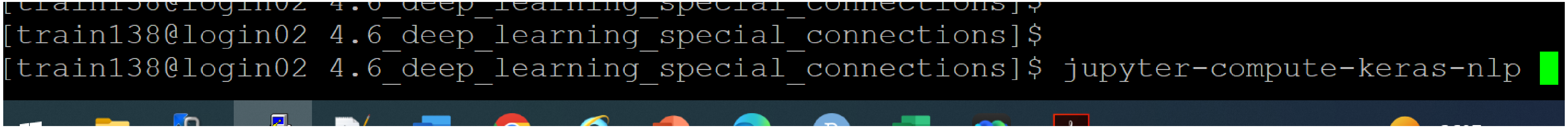


Notebook exercise using KerasNLP

- In a terminal window start the notebook session for keras-nlp

  …]$ cd 4.6_deep_learning_special_connections

  …]$ jupyter-compute-keras-nlp



- Open the URL and look for the *CIML23_BERT_FineTune_v3.ipynb* notebook

Keras NLP package has several BERT versions

So let's start with 'bert-small' (28M parameters)

For reference:
$\text{BERT}_{\text{BASE}}$ (L=12, H=768, Attn=12, Total Parameters=110M)
$\text{BERT}_{\text{LARGE}}$ (L=24, H=1024, Attn=16, Total Parameters=340M).

models/

bert_tiny_en_uncased	BERT	4M	2-layer BERT model where all input is lowercased. Trained on English Wikipedia + BooksCorpus.
bert_small_en_uncased	BERT	28M	4-layer BERT model where all input is lowercased. Trained on English Wikipedia + BooksCorpus.
bert_medium_en_uncased	BERT	41M	8-layer BERT model where all input is lowercased. Trained on English Wikipedia + BooksCorpus.
bert_base_en_uncased	BERT	109M	12-layer BERT model where all input is lowercased. Trained on English Wikipedia + BooksCorpus.
bert_base_en	BERT	108M	12-layer BERT model where case is maintained. Trained on English Wikipedia + BooksCorpus.
bert_base_zh	BERT	102M	12-layer BERT model. Trained on Chinese Wikipedia.
bert_base_multi	BERT	177M	12-layer BERT model where case is maintained. Trained on trained on Wikipedias of 104 languages

END