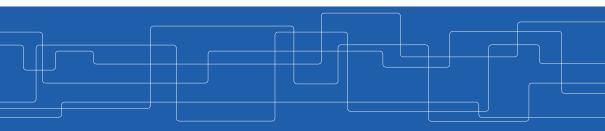


RNNs and Transformers

Jim Dowling jdowling@kth.se 2022-11-23

Slides by Francisco J. Pena, Amir H. Payberah, and Jim Dowling



Language Modeling (1/2)

▶ Language modeling is the task of predicting what word comes next.





Language Modeling (2/2)

▶ More formally: given a sequence of words $x^{(1)}, x^{(2)}, \dots, x^{(t)}$, compute the probability distribution of the next word $x^{(t+1)}$:

$$p(x^{(t+1)} = w_j | x^{(t)}, \cdots x^{(1)})$$

ightharpoonup w_j is a word in vocabulary $V = \{w_1, \dots, w_v\}$.



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.
 - Unigrams: "the", "students", "opened", "their"
 - Bigrams: "the students", "students opened", "opened their"
 - Trigrams: "the students opened", "students opened their"
 - 4-grams: "the students opened their"
- ► Collect statistics about how frequent different n-grams are, and use these to predict next word.



n-gram Language Models - Example

- ► Suppose we are learning a 4-gram Language Model.
 - $x^{(t+1)}$ depends only on the preceding 3 words $\{x^{(t)}, x^{(t-1)}, x^{(t-2)}\}$.

```
p(w_j|students\ opened\ their) = \frac{\text{students\ opened\ their}}{\text{students\ opened\ their}}
```

- ▶ In the corpus:
 - "students opened their" occurred 1000 times
 - "students opened their books occurred 400 times: p(books|students opened their) = 0.4
 - "students opened their exams occurred 100 times: p(exams|students|opened|their) = 0.1



Problems with n-gram Language Models - Sparsity

$$p(w_j|students opened their) = \frac{students opened their w_j}{students opened their}$$

- ▶ What if "students opened their w_j " never occurred in data? Then w_j has probability 0!
- ► What if "students opened their" never occurred in data? Then we can't calculate probability for any w_j!
- ▶ Increasing n makes sparsity problems worse.
 - Typically we can't have n bigger than 5.



Problems with n-gram Language Models - Storage

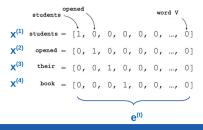
$$p(w_j|students opened their) = \frac{students opened their w_j}{students opened their}$$

- ▶ For "students opened their w_j ", we need to store count for all possible 4-grams.
- ▶ The model size is in the order of $O(\exp(n))$.
- ► Increasing n makes model size huge.



Can We Build a Neural Language Model? (1/3)

- ► Recall the Language Modeling task:
 - Input: sequence of words $x^{(1)}, x^{(2)}, \dots, x^{(t)}$
 - Output: probability dist of the next word $p(x^{(t+1)} = w_1 | x^{(t)}, \dots, x^{(1)})$
- ▶ One-Hot encoding
 - Represent a categorical variable as a binary vector.
 - All recodes are zero, except the index of the integer, which is one.
 - Each embedded word $e^{(t)} = E^T x^{(t)}$ is a one-hot vector of size vocabulary size.

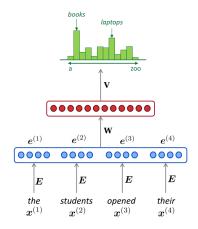




Can We Build a Neural Language Model? (2/3)

► A MLP model

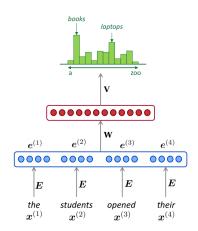
- Input: words $x^{(1)}, x^{(2)}, x^{(3)}, x^{(4)}$
- Input layer: one-hot vectors $\mathbf{e}^{(1)}$, $\mathbf{e}^{(2)}$, $\mathbf{e}^{(3)}$, $\mathbf{e}^{(4)}$
- Hidden layer: $\mathbf{h} = \mathbf{f}(\mathbf{w}^{\mathsf{T}}\mathbf{e})$, \mathbf{f} is an activation function.
- Output: $\hat{\mathbf{y}} = \text{softmax}(\mathbf{v}^{\mathsf{T}}\mathbf{h})$





Can We Build a Neural Language Model? (3/3)

- ► Improvements over n-gram LM:
 - No sparsity problem
 - Model size is O(n) not O(exp(n))
- ► Remaining problems:
 - It is fixed 4 in our example, which is small
 - We need a neural architecture that can process any length input





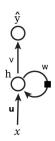
Recurrent Neural Networks (RNN)

- ► The idea behind Recurrent neural networks (RNN) is to make use of sequential data.
 - Until here, we assume that all inputs (and outputs) are independent of each other.
 - Independent input (output) is a bad idea for many tasks, e.g., predicting the next word in a sentence (it's better to know which words came before it).
- ► They can analyze time series data and predict the future.
- ► They can work on sequences of arbitrary lengths, rather than on fixed-sized inputs.



Recurrent Neural Networks (2/4)

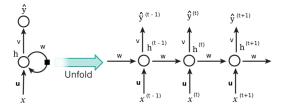
- ▶ Neurons in an RNN have connections pointing backward.
- ► RNNs have memory, which captures information about what has been calculated so far.





Recurrent Neural Networks (3/4)

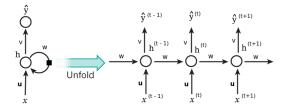
- ▶ Unfolding the network: represent a network against the time axis.
 - We write out the network for the complete sequence.
- ► For example, if the sequence we care about is a sentence of three words, the network would be unfolded into a 3-layer neural network.
 - One layer for each word.





Recurrent Neural Networks (4/4)

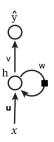
- $\mathbf{h}^{(t)} = \mathbf{f}(\mathbf{u}^{\mathsf{T}}\mathbf{x}^{(t)} + \mathbf{w}\mathbf{h}^{(t-1)})$, where f is an activation function, e.g., tanh or ReLU.
- $\hat{y}^{(t)} = g(vh^{(t)})$, where g can be the softmax function.
- $\blacktriangleright \ \text{cost}(\textbf{y}^{(t)}, \boldsymbol{\hat{y}}^{(t)}) = \text{cross_entropy}(\textbf{y}^{(t)}, \boldsymbol{\hat{y}}^{(t)}) = -\sum \textbf{y}^{(t)} \text{log} \boldsymbol{\hat{y}}^{(t)}$
- $ightharpoonup y^{(t)}$ is the correct word at time step t, and $\hat{y}^{(t)}$ is the prediction.





Recurrent Neurons - Weights (1/4)

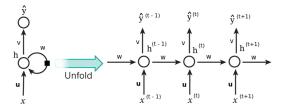
► Each recurrent neuron has three sets of weights: **u**, **w**, and **v**.





Recurrent Neurons - Weights (2/4)

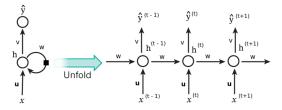
- ▶ **u**: the weights for the inputs **x**^(t).
- ► x^(t): is the input at time step t.
- ► For example, **x**⁽¹⁾ could be a one-hot vector corresponding to the first word of a sentence.





Recurrent Neurons - Weights (3/4)

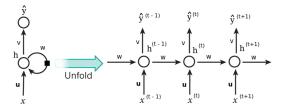
- \triangleright w: the weights for the hidden state of the previous time step $h^{(t-1)}$.
- ▶ h^(t): is the hidden state (memory) at time step t.
 - $h^{(t)} = tanh(\mathbf{u}^\mathsf{T}\mathbf{x}^{(t)} + wh^{(t-1)})$
 - h⁽⁰⁾ is the initial hidden state.





Recurrent Neurons - Weights (4/4)

- v: the weights for the hidden state of the current time step h^(t).
- $ightharpoonup \hat{\mathbf{y}}^{(t)}$ is the output at step t.
- $\mathbf{\hat{y}}^{(t)} = softmax(vh^{(t)})$
- ► For example, if we wanted to predict the next word in a sentence, it would be a vector of probabilities across our vocabulary.

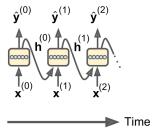


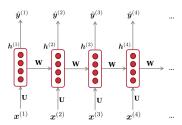


Layers of Recurrent Neurons

At each time step t, every neuron of a layer receives both the input vector $\mathbf{x}^{(t)}$ and the output vector from the previous time step $\mathbf{h}^{(t-1)}$.

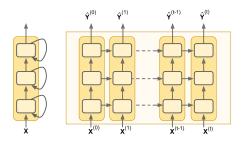
$$\begin{aligned} \mathbf{h}^{(\texttt{t})} &= \texttt{tanh}(\mathbf{u}^{\intercal}\mathbf{x}^{(\texttt{t})} + \mathbf{w}^{\intercal}\mathbf{h}^{(\texttt{t}-1)}) \\ \mathbf{y}^{(\texttt{t})} &= \texttt{sigmoid}(\mathbf{v}^{\intercal}\mathbf{h}^{(\texttt{t})}) \end{aligned}$$







► Stacking multiple layers of cells gives you a deep RNN.



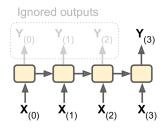


RNN Design Patterns



RNN Design Patterns - Sequence-to-Vector

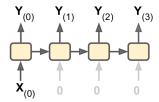
- ► Sequence-to-vector network: takes a sequence of inputs, and ignore all outputs except for the last one.
- ► E.g., you could feed the network a sequence of words corresponding to a movie review, and the network would output a sentiment score.





RNN Design Patterns - Vector-to-Sequence

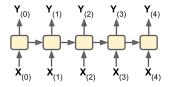
- ▶ Vector-to-sequence network: takes a single input at the first time step, and let it output a sequence.
- ► E.g., the input could be an image, and the output could be a caption for that image.





RNN Design Patterns - Sequence-to-Sequence

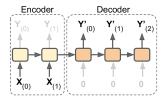
- ► Sequence-to-sequence network: takes a sequence of inputs and produce a sequence of outputs.
- ▶ Useful for predicting time series such as stock prices: you feed it the prices over the last N days, and it must output the prices shifted by one day into the future.
- ▶ Here, both input sequences and output sequences have the same length.





RNN Design Patterns - Encoder-Decoder

- ► Encoder-decoder network: a sequence-to-vector network (encoder), followed by a vector-to-sequence network (decoder).
- ► E.g., translating a sentence from one language to another.
- ▶ You would feed the network a sentence in one language, the encoder would convert this sentence into a single vector representation, and then the decoder would decode this vector into a sentence in another language.



- Sometimes we only need to look at recent information to perform the present task.
 - E.g., predicting the next word based on the previous ones.
- ▶ In such cases, where the gap between the relevant information and the place that it's needed is small, RNNs can learn to use the past information.
- ▶ But, as that gap grows, RNNs become unable to learn to connect the information.
- ► RNNs may suffer from the vanishing/exploding gradients problem.

- ▶ Ian Goodfellow et al., Deep Learning (Ch. 10)
- ► Aurélien Géron, Hands-On Machine Learning (Ch. 15)
- Understanding LSTM Networks http://colah.github.io/posts/2015-08-Understanding-LSTMs
- ► CS224d: Deep Learning for Natural Language Processing http://cs224d.stanford.edu

Problem: Word embeddings are context-free



walk	to	the	bank	and	get	cash
0.02	0.01	-0.04	-0.02	-0.02	-0.06	0.01
:	:	:	:	:	:	:
-0.07	0.02	-0.03	-0.03	0.02	0.04	-0.01

[Peltarion, 2020]



Problem: Word embeddings are context-free



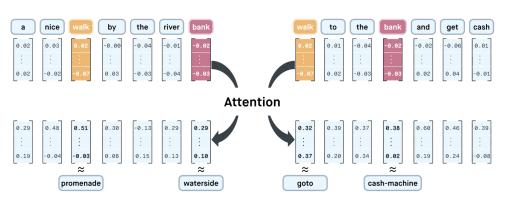


[Peltarion, 2020]



Word Embeddings

Problem: Word embeddings are context-free **Solution:** Create contextualized representation



[Peltarion, 2020]



From RNNs to Transformers



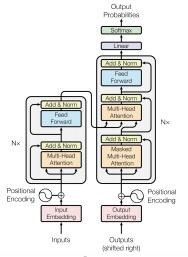
Problems with RNNs - Motivation for Transformers

- Sequential computations prevents parallelization
- ► Despite GRUs and LSTMs, RNNs still need attention mechanisms to deal with long range dependencies
- ▶ Attention gives us access to any state...Maybe we don't need the costly recursion?
- ▶ Then NLP can have deep models, solves our computer vision envy!



Attention is all you need! [Vaswani, 2017]

- ► Sequence-to-sequence model for Machine Translation
- ► Encoder-decoder architecture
- ► Multi-headed self-attention
 - Models context and no locality bias



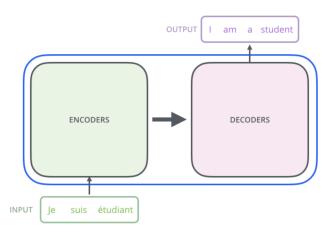
[Vaswani et al., 2017]



Transformers Step-by-Step



Understanding the Transformer: Step-by-Step



[Alammar, 2018]



Understanding the Transformer: Step-by-Step

No recursion, instead stacking encoder and decoder blocks

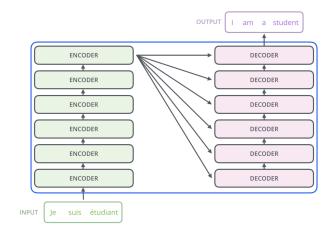
► Originally: 6 layers

▶ BERT base: 12 layers

▶ BERT large: 24 layers

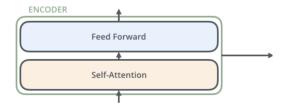
► GPT2-XL: 48 layers

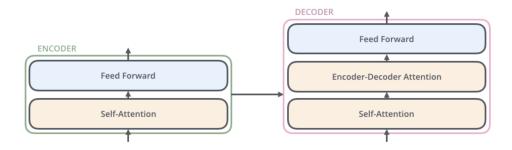
► GPT3: 96 layers



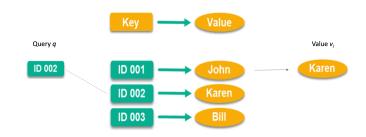


The Encoder and Decoder Blocks





Mimics the retrieval of a value v_i for a query q based on a key k_i in a database, but in a probabilistic fashion



Dot-Product Attention

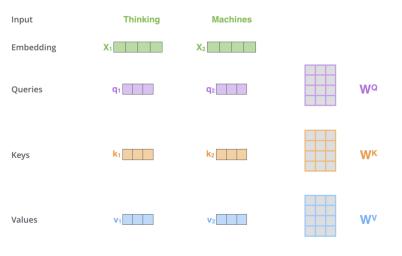
- Queries, keys and values are vectors
- Output is a weighted sum of the values
- Weights are are computed as the scaled dot-product (similarity) between the query and the kevs

Attention
$$(q, K, V) = \sum_{i} \text{Similarity}(q, k_i) \cdot v_i = \sum_{i} \frac{e^{q \cdot k_i / \sqrt{d_k}}}{\sum_{j} e^{q \cdot k_j / \sqrt{d_k}}} v_i$$
 Output is a row-vector

- Can stack multiple queries into a matrix Q Attention $(Q, K, V) = \operatorname{softmax} \left(\frac{QK^{\top}}{\sqrt{d_{\nu}}} \right) V$ Output is again a matrix
- Self-attention: Let the word embeddings be the queries, keys and values, i.e. let the words select each other

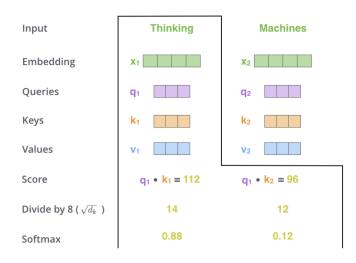


Self-Attention Mechanism



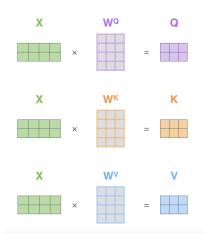


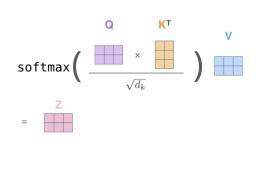
Self-Attention Mechanism





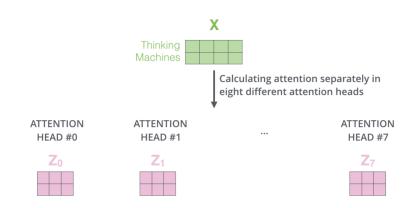
Self-Attention Mechanism in Matrix Notation





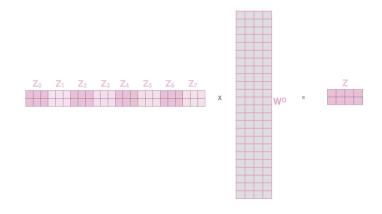


Multi-Headed Self-Attention



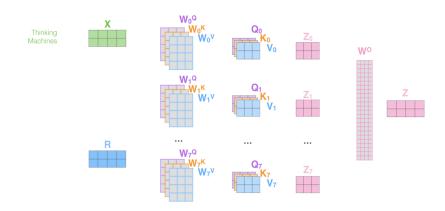


Multi-Headed Self-Attention

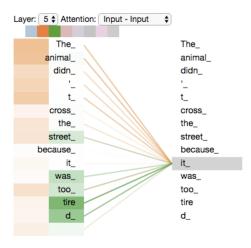




Self-Attention: Putting It All Together





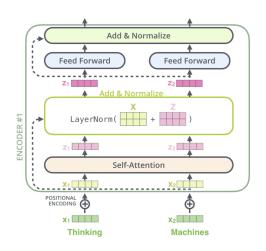




The Full Encoder Block

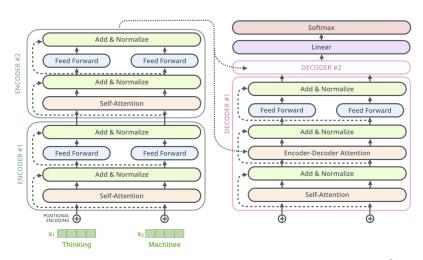
Encoder block consisting of:

- Multi-headed self-attention
- ► Feedforward NN (FC 2 layers)
- Skip connections
- Layer normalization Similar to batch normalization but computed over features (words/tokens) for a single sample





Encoder-Decoder Architecture - Small Example





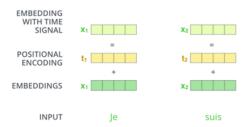
Positional Encodings

Encoder block consisting of:

- ► Attention mechanism has no locality bias no notion of word order
- Add positional encodings to input embeddings to let model learn relative positioning

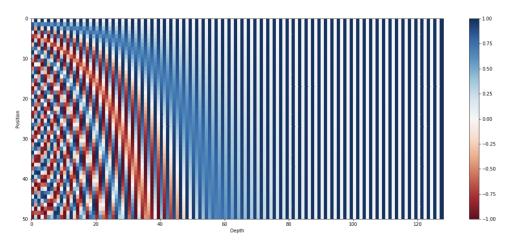
$$\mathsf{PE}(\mathsf{pos},2i) = \sin\left(\frac{\mathsf{pos}}{10000^{2i/d_{\mathsf{model}}}}\right)$$

$$\mathsf{PE}(\mathsf{pos}, 2i + 1) = \cos\left(\frac{\mathsf{pos}}{10000^{2i/d_{\mathsf{model}}}}\right)$$





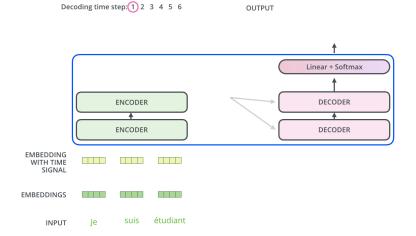
Positional Encodings



[Kazemnejad, 2019]



Let's start the encoding!





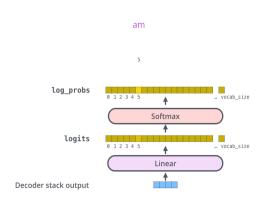
Decoding time step: 1 (2) 3 4 5 6 OUTPUT Linear + Softmax Kencdec Vencdec **ENCODERS** DECODERS **EMBEDDING** WITH TIME SIGNAL **EMBEDDINGS PREVIOUS** suis étudiant INPUT OUTPUTS



Producing the output text

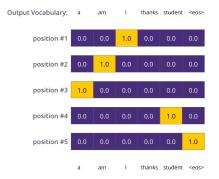
Encoder block consisting of:

- ► The output from the decoder is passed through a final fully connected linear layer with a softmax activation function
- Produces a probability distribution over the pre-defined vocabulary of output words (tokens)
- Greedy decoding picks the word with the highest probability at each time step

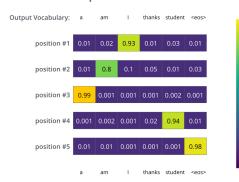




Target Model Outputs



Trained Model Outputs





Layer Type	Complexity per Layer	Sequential	Maximum Path Length	
		Operations		
Self-Attention	$O(n^2 \cdot d)$	O(1)	O(1)	
Recurrent	$O(n \cdot d^2)$	O(n)	O(n)	
Convolutional	$O(k \cdot n \cdot d^2)$	O(1)	$O(log_k(n))$	

[Vaswani et al., 2017]



Model	BLEU		Training C	Training Cost (FLOPs)	
Wiodei	EN-DE	EN-FR	EN-DE	EN-FR	
ByteNet [15]	23.75				
Deep-Att + PosUnk [32]		39.2		$1.0 \cdot 10^{20}$	
GNMT + RL [31]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$	
ConvS2S [8]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$	
MoE [26]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$	
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0 \cdot 10^{20}$	
GNMT + RL Ensemble [31]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$	
ConvS2S Ensemble [8]	26.36	41.29	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$	
Transformer (base model)	27.3	38.1	3.3	$3.3\cdot 10^{18}$	
Transformer (big)	28.4	41.0	2.3	$2.3 \cdot 10^{19}$	

[Vaswani et al., 2017]



BERT



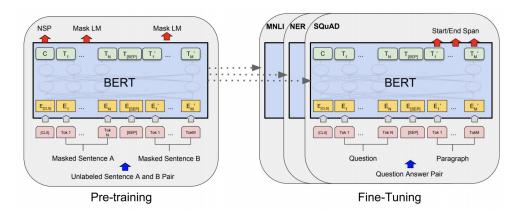
Bidirectional Encoder Representations from Transformers

- Self-supervised pre-training of Transformers encoder for language understanding
- ► Fine-tuning for specific downstream task





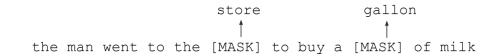
BERT Training Procedure



[Devlin et al., 2018]



Masked Language Modelling



Next Sentence prediction

Sentence A = The man went to the store.

Sentence B = He bought a gallon of milk.

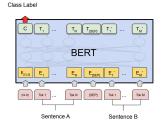
Label = IsNextSentence

Sentence A = The man went to the store.
Sentence B = Penguins are flightless.
Label = NotNextSentence

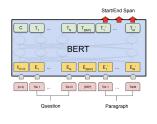
[Devlin et al., 2018]



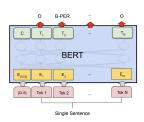
Sentence Classification



Question Answering



Named Entity Recognition



[Devlin et al., 2018]



How good are transformers?

- ► Scaling up models size and amount of training data helps a lot
- ▶ Best model is 10B (!!) parameters
- ▶ Two models have already surpassed human performance!!!
- Exact pre-training objective (MLM, NSP, corruption) doesn't matter too much
- ► SuperGLUE benchmark:



[Raffel et al., 2019]



Practical Examples

GOOGLE TECH ARTIFICIAL INTELLIGENCE

Google is improving 10 percent of searches by understanding language context

Say hello to BERT

By Dieter Bohn | @backlon | Oct 25, 2019, 3:01am EDT

Bing says it has been applying BERT since April

The natural language processing capabilities are now applied to all Bing queries globally.

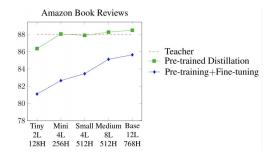
George Nguyen on November 19, 2019 at 1:38 pm

[Devlin, 2020]



Distillation

- Modern pre-trained language models are huge and very computationally expensive
- How are these companies applying them to low-latency applications?
- ▶ Distillation!
 - Train SOTA teacher model (pre-training + fine-tuning)
 - Train smaller student model that mimics the teacher's output on a large dataset on unlabeled data
- ➤ Distillation works *much* better than pre-training + fine-tuning with smaller model



[Devlin, 2020] [Turc, 2020]



Transformers in TensorFlow using HuggingFace (2)





1. Back to home

All Models and checkpoints



- ► The HuggingFace Library contains a majority of the recent pre-trained State-of-the-art NLP models, as well as over 4 000 community uploaded models
- Works with both TensorFlow and PyTorch



Transformers in TensorFlow using HuggingFace



```
from transformers import BertTokenizerFast, TFBertForSequenceClassification
from datasets import load dataset
import tensorflow as tf
dataset = load dataset("imdb").shuffle()
tokenizer = BertTokenizerFast.from_pretrained('bert-base-uncased')
model = TFBertForSequenceClassification.from_pretrained('bert-base-uncased', num_labels=2)
train_encodings = tokenizer(dataset['train']['text'], truncation=True, padding=True)
train dataset = tf.data.Dataset.from tensor slices((dict(train encodings), dataset['train']['label']))
val dataset = ... // Analogously
optimizer = tf.keras.optimizers.Adam(learning rate=5e-5)
model.compile(optimizer=optimizer, loss=model.compute_loss)
model.fit(train dataset.batch(16), epochs=3, batch size=16)
model.evaluate(val dataset.batch(16), verbose=0)
```



Transformers in TensorFlow using HuggingFace 🤗

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Transformers in TensorFlow using HuggingFace 🤗

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Transformers in TensorFlow using HuggingFace 🤗

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Wrap Up

KTH Summary

- Transformers have blown other architectures out of the water for NLP
- Get rid of recurrence and rely on self-attention
- ► NLP pre-training using Masked Language Modelling
- Most recent improvements using larger models and more data
- ▶ Distillation can make model serving and inference more tractable

