

Image: Transformers: ' ... and one 'architecture' to rule them all' - Juxtaposition by Raeid Saqur (2024).

Transformers

CSC401/2511 – Natural Language Computing – Winter 2024 Gerald Penn, Sean Robertson & Raeid Saqur



UNIVERS Lecture 6 University of Toronto



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1

Logistics (Feb 12, 2024)

- Office hours: Mon 12 13.00 (in-person, BA 2270)
- A2 is now posted! due Mar 8, 2024 (mid-night) errata recap.
- A2 tutorials planned schedule:
 - Feb 16: A2 tutorial 1 (ft. Arvid Frydenlund)
 - Mar 1: A2 tutorial 2 (ft. Julia Watson)
 - Mar 8: A2 Q/A and OH
- A3: release Mar 9, 2024
- Final exam: date to be finalized soon
- Have a great Reading week break! Next week: no classes or tutorials).
- Lecture feedback:
 - Anonymous
 - Please share any thoughts/suggestions

• Questions?





A2 – NMT with Transformers

Tacks	Section	Class	critorion	Max mark	Sub-	File
IdSKS	Section	LaverNorm	ferward		Total	rile
1	Puilding	LayerNorm	intraction	2		
2	Building	MultiHeadAttention	ferward	4		
3	BIOCKS	FoodForwardLavor	forward	5	12	
4	e lectroi wai uLayei		.ioiward	2	12	
5		TransformerEncoderLayer	:pre_layer_norm_forward	2		
7			:post_layer_norm_forward	1		
/		TransformerDecederlayer	:Init	4		
8	Architocture	Transformer Decoder Layer	:pre_layer_norm_forward	2		
9	Architecture	TransformerDeceder	:post_layer_norm_forward	2		2 townsformer medal m
10		TransformerDecoder	:torward	3		a2_transformer_model.py
11		T	:create_pad_mask	1		
12		TransformerEncoderDecoder	:create_causal_mask	2	-	
13			:forward	3	20	
15			:greedy_decode	5		-
17	Decoding:		: expand_encoder_for_beam_search	3		-
18	Greedy, and	TransformerEncoderDecoder	: repeat_and_reshape_for_beam_search	1		-
19	beam-search		: initialize_beams_for_beam_search	6		-
20				: pad_and_score_sequence_for_beam_search	3	
21			:finalize_beams_for_beam_search 2		20	
22			:train_input_target_split	1		-
23	Training		:train_step_optimizer_and_scheduler	1		
24	and	TransformerRunner	:train_for_epoch	5		a2_transformer_runner.py
25	testing		:translate	2		
26			:compute_batch_total_bleu	3	12	
27			BLEU score: grouper	2		
28	BLEU		BLEU score: n_gram_precision	2		a2 blau scora pu
29	score		BLEU score: brevity_penalty	2		uz_bieu_score.py
30			BLEU score: BLEU_Score()	2	8	
32	Analysis			8	8	analysis.pdf

Transformers

Lecture plan (L6)

- Overview/Recap: RNNs -> Transformers
- Transformer building blocks/components
- Transformer architecture deep dive
- Review of early popular Transformer based PLMs:
 - Encoder only (BERT, BERTology findings)
 - Encoder-Decoder: unified text-to-text format (T5)
 - Decoder only auto-regressive models (GPT)
- What's next for LM architectures?
 - Token free architectures
 - Is Attention all we need? Attention free architectures
- Segue to the next lecture (L7) LLMs



Transformer networks

- Breakout paper in 2017: Attention is all you need [1]
- **Core idea**: replace recurrent connections with attention

Madal	BL	EU	Training Cost (FLOPs		
Model	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	$9.6\cdot10^{18}$	$1.5\cdot 10^{20}$	
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 •	10^{18}	
Transformer (big)	28.4	41.0	$2.3 \cdot$	10^{19}	

Empirical results showcased using machine translation (WMT'14)

¹ Vaswani, Ashish, et al. "Attention is all you need." NeuIPS (2017).



Transformer networks (abstract)

*Recall Slide

t = 1 ... T



Transformer motivations

- Limitations of recurrent connections: long-term dependencies, lack of parallelizability, interaction distance (steps to distant tokens).
- Attention allows access to entire sequence
- Lots of computation can be shared, parallelized across sequence indices. Identical layers: [self, cross]-attention, feed-forward w/ tricks
 - Layer norm., residual connections, positional encodings, masking
 - See Vaswani et al (2017) for specific architecture



Source sentence (French): *L' amitié est magique* Target sentence (English): *Friendship is magic*



RNNs to Transformers

- **Transformers** is the underlying architecture for all state-of-the-art deep neural models – not just in NLP, but across other modalities too
- So far, we have seen encoder-decoder models using RNN (and variant) • architectures using *attention* for memory bottlenecks (*seq2seq+attn*)



- With Transformers, we use the same (enc-dec) paradigm, with different building blocks Encoder Decoder
 - by removing recurrence with parallelizable blocks

¹Vaswani, Ashish, et al. "Attention is all you need." *NeuIPS* (2017).



 i_{t-1}



- Architecture diagram from Vaswani^[1]
- Building blocks:
 - 1. Encoder
 - 2. Decoder



¹ Vaswani, Ashish, et al. "Attention is all you need." *NeuIPS* (2017).







- Architecture diagram from Vaswani^[1]
- Building blocks:
 - 1. Encoder
 - 2. Decoder
- Main components within building blocks:
 - Attention mechanisms:
 - single and multi-head attention
 - self, cross, and masked attention
 - Feed-forward MLPs (FFN)
 - Layer normalization (LN)
 - Positional encodings (PE)
 - Residual connections

¹ Vaswani, Ashish, et al. "Attention is all you need." NeuIPS (2017).





Transformer Attention(Q,K,V): Intuition

In the classical roboquity era (2100-2250 AD), humans in designated zones/zoos are only allowed *filing cabinets* and *paper documents* to store information.

ACORN doesn't exist, and UofT students' info (financial, academic, personal) retrieval works as follows:



MatMul

Scale MatMu

Transformer Encoder



- 1. Residual connections
- 2. LayerNorm
- 3. Attention and FFN sub-layers
- 4. Positional encodings



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Residual Connections



- **Problem**: NNs struggle to learn the identity function mapping
- Solution: Add back the input embeddings to the sub-layer's output moving up $x'_{s} = Sublayer(x_{s}) + x_{s}$
- *Analogy*: think of the information highway analogy. Helps negate forgetting past information by carrying information without distortion.

¹He, Kaiming, et al. "Deep residual learning for image recognition." *CVPR*. 2016.



Layer Normalization: default (Post-) LN



$$\frac{\mathbf{h^{l'}} = LayerNorm(\mathbf{h^{l}}) }{= \gamma\left(\frac{\mathbf{h^{l}} - \mu^{l}}{\sigma^{l}}\right) + \beta }$$

where μ , σ are mean and std. dev. of features in h^l . γ , β are scale, bias params.

$$\mu = \frac{1}{d} \sum_{k=1}^{d} h_k^l$$
$$\sigma^2 = \frac{1}{d} \sum_{k=1}^{d} (h_k^l - \mu)^2$$

- Layer Normalization^[1]:
 - Normalize input layer's distribution to 0 mean and 1 standard deviation.
 - Removes uninformative variation in layer's features

¹Ba, Jimmy Lei, Jamie Ryan Kiros, and Geoffrey E. Hinton. "Layer normalization. 2016" [link]
 ²Xiong, Ruibin, et al. "On layer normalization in the transformer architecture." *ICML*. PMLR, 2020. [link]



Layer Normalization Variant: Pre-LN



- Layer Normalization^[1]: two popular variants
 - Post layer normalization (Post-LN): original Transformer model: requires learning rate warm-up due to initial instability of large output gradients.
 - *Pre layer normalization* (Pre-LN): puts layer-norm within the residual block. Allows removing warm-up stage. More stable training initialization.

¹Ba, Jimmy Lei, Jamie Ryan Kiros, and Geoffrey E. Hinton. "Layer normalization. 2016" [link] ²Xiong, Ruibin, et al. "On layer normalization in the transformer architecture." *ICML*. PMLR, 2020. [link]

E_T:

Add & Norm Feed Forward N× Add & Norm Multi-Head Attention Positional Encoding χ_{2} Input F_S: Mini tutoriel de Embeddina transformateur </s>Inputs

Tiny transformer tutorial

• Our running example:

- Three weight matrices W^Q, W^K, W^V
- Let's look at 'self-attention' with input F_{S}

¹ Vaswani, Ashish, et al. "Attention is all you need." NeuIPS (2017).

- Recall the attention steps we discussed in last lecture
- Steps:
 - 1. Calculate the query, key, and value for each token
 - Attention of each query (q_i) against all the keys $(k_{1:i})$
 - 2. Calculate the **attention score** between query and keys
 - 3. Normalize the attention scores by applying softmax
 - 4. Calculate values by taking a weighted sum

$$\begin{array}{c} \boldsymbol{q}_{i} = W^{Q} \boldsymbol{x}_{i} \\ \boldsymbol{k}_{i} = W^{K} \boldsymbol{x}_{i} \\ \boldsymbol{v}_{i} = W^{V} \boldsymbol{x}_{i} \end{array} \qquad \begin{array}{c} a_{i,j} = score(\boldsymbol{q}_{i}, \boldsymbol{k}_{j}) \\ a_{i,j} = \boldsymbol{q}_{i}. \boldsymbol{k}_{j} \\ a_{i,j} = \frac{\boldsymbol{q}_{i}. \boldsymbol{k}_{j}}{\sqrt{d_{k}}} \end{array} \qquad \begin{array}{c} \alpha_{i,j} = softmax(\boldsymbol{a}_{i,1:K}) \\ \alpha_{i,j} = softmax(\boldsymbol{a}_{i,j}) \\ \alpha_{i,j} = \frac{exp^{(a_{i,j})}}{\sum_{k=1}^{K} exp^{(a_{i,k})}} \end{array} \qquad \begin{array}{c} c_{i} = \sum_{j} \alpha_{i,j} \boldsymbol{v}_{j} \end{array}$$

¹ Vaswani, Ashish, et al. "Attention is all you need." NeuIPS (2017).

- Recall the attention steps we discussed in last lecture
- Steps:
 - 1. Calculate the query, key, and value for each token
 - Attention of each query (q_i) against all the keys $(k_{1:i})$ •
 - 2. Calculate the **attention score** between query and keys
 - **Normalize** the attention scores by applying softmax 3.
 - 4. Calculate values by taking a weighted sum

Vectorized notation:

$$Q = XW^{Q}$$

$$K = XW^{K}$$

$$K = XW^{K}$$

$$V = XW^{V}$$

$$A = Q.K^{T}$$

$$A = Q.K^{T}$$

$$A = softmax(\frac{QK^{T}}{\sqrt{d_{k}}})$$

$$Z = A.V$$

¹Vaswani, Ashish, et al. "Attention is all you need." *NeuIPS* (2017).

N×

Add & Norr Feed Forward

Multi-head Self Attention (MHA)

 As alluded to in L5, multi-head attention (MHA) allows to jointly attend to information from different representation subspaces at different positions

> $MHA(Q, K, V) = Concat(head_1, ..., head_h)W^{O}$ where head_i = Attention(QW_i^Q, KW_i^K, VW_i^V) And projections are parameter matrices:

$$W_{i}^{Q} \in \mathbb{R}^{d_{model} \times d_{k}} \qquad W^{O} \in \mathbb{R}^{hd_{v} \times d_{model}}$$
$$W_{i}^{K} \in \mathbb{R}^{d_{model} \times d_{k}} \qquad d_{k} = d_{v} = \frac{d_{model}}{h}$$

¹ Vaswani, Ashish, et al. "Attention is all you need." NeuIPS (2017).

Feed-forward (FFN) layers

- Attention only re-weighs the value vectors
- We need to apply *non-linearities* (activations) to enable (deep) learning
- The feed-forward layer(s) (FFN) provide non-linear activation to attention layer outputs
- Specifically, each output x undergoes two (layer) linear transformations with a ReLU activation in between:

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

- FFN sub-layer is applied to each token pos. separately and identically
- Given x is a sequence of tokens (x₁, ..., x_S), point-wise computation of FFN sub-layer on any token x_i is:

$$FFN(x_i) = ReLU(x_iW_1 + b_1)W_2 + b_2$$

where W_1 , W_2 , b_1 and b_2 are parameters

¹ Vaswani, Ashish, et al. "Attention is all you need." *NeuIPS* (2017).

Position (in)dependence

- Attention mechanism is agnostic to sequence order
 - For permutation vector v s.t. sorted(v) = (1, 2, ..., V)

 $Att(a, b_{v}) = Att(a, b_{1:V})$

- Caveat: but the word order matters in language translation
- **Solution**: encode position in input:

$$x_s = T_F(F_s) + \phi(s)$$

Transformer - Positional Encoding

*Recall slide: L5_NMT

Add positional information of an input token in the sequence into the input embedding vectors.

$$PE_{(pos, 2i)} = \sin\left(\frac{pos}{10000^{\left(\frac{2i}{d_{model}}\right)}}\right); PE_{(pos, 2i+1)} = \cos\left(\frac{pos}{10000^{\left(\frac{2i}{d_{model}}\right)}}\right)$$

- The *positional encodings* (PE) have the same dimension d_{model} as the embeddings (for summation)
- Many choices of PEs possible: learned or fixed.

Recap: Transformer Architecture

- Architecture diagram from Vaswani^[1]
- Building blocks:
- 🗹 1. Encoder
 - 2. <mark>Decoder</mark>
- Main components within building blocks:
 - Attention mechanisms:
 single and multi-head attention
 - self, cross, and masked attention
- Feed-forward MLPs (FFN)
 - Layer normalization (LN)
 - Positional encodings (PE)
 - Residual connections

Next block: Transformer Decoder

- Layer normalization, residual connections, FFNs are identical to the encoder block
- Thus, we focus on remaining:
 - Masked/Causal self-attention sub-layer
 - Cross-attention

¹ Vaswani, Ashish, et al. "Attention is all you need." *NeuIPS* (2017).

Decoder – Masked Self-Attention

- Masked (Multi-head) self-attention:
 - Enforce auto-regressive language modeling objective. The decoder cannot peek and pay attention to the (unknown) future words
 - Solution: use a look-head mask M, by setting attention scores of future tokens to –inf.

$$a_{ij} = \begin{cases} q_i^T \cdot k_j, j < i \\ -\infty, j \ge i \end{cases}$$

¹ Vaswani, Ashish, et al. "Attention is all you need." NeuIPS (2017).

Decoder – Masked Self-Attention

Encoder-Decoder (Cross) Attention

- In self-attention: Q, K and V has same source (tokens)
- Cross attention is encoder <> decoder attention between encoder and decoder's output vectors (like we are used to from L5-NMT
- Using our running e.g. and notations:
 - Let h_1, \ldots, h_S be encoder output vectors, where $h_i \in \mathbb{R}^{d_k}$
 - Let $\tilde{h}_1, \dots, \tilde{h}_T$ be decoder output vectors, where $\tilde{h}_i \in \mathbb{R}^{d_q}$
- Then, keys and values: K and V comes from encoder (or, memory):
 - $k_i = Kh_i$, $v_i = Vh_i$
- Queries, **Q** comes from decoder:

• $q_i = \frac{Q}{\tilde{h}_i}$

Encoder-Decoder (Cross) Attention

(Compare) Encoder - Self Attention

Recap

- We have now covered all the primitives you need for building a transformer!
- These are too abstract, but not to worry ...
- Assignment 2 was designed for you to implement all these concepts into a working MT model of your own!

			Class			Sub-	
	Tasks	Section	0.035	criterion	Max mark	Total	File
	1		LayerNorm	:forward	2		
	2	Building	MultiHeadAttention	:attention	4		
	3	Blocks	MultineauAttention	:forward	5		
	4		FeedForwardLayer	:forward	1	12	
	5		TransformerEncoderLover	:pre_layer_norm_forward	2		
	6		Transformer Encoder Layer	:post_layer_norm_forward	1		
	7			:init	4		
	8		TransformerDecoderLayer	:pre_layer_norm_forward	2		
	9	Architecture		:post_layer_norm_forward	2		
	10		TransformerDecoder	:forward	3		a2_transformer_model.py
	11			:create_pad_mask	1		
	12		TransformerEncoderDecoder	:create_causal_mask	2		
	13			:forward	3	20	
_	15			igraadu dacada	E		

Transformers - Drawbacks

- Attention's quadratic computation cost
 - Function of sequence length N, and token dimension d
 - Computing all token pairs mean the function grows quadratically with N, $O(N^2d)$ unlike RNNs: O(Nd)

 Can you see why this could be the biggest hurdle for increasing a transformer LM's context length (i.e., the size of input it can process)?

Transformers - Drawbacks

- Context (input) size limitation:
 - Dimension d in modern LLMs are ~>3K
 - If one sentence length is ~10-30 word tokens, then computation scales with 10²-30² times d
 - Thus, modern LLMs set a bound on N (usually 512 tokens)
 - But, we want **N** to be much larger
 - E.g., processing a document (N > 10K) at one go (instead of chunking by N for every call)
- Active research area: improving the quadratic cost of attention, like self-attention with linear complexity^[1]
 - + Roformer, flash attention, sliding-window etc.

[1] Wang, Sinong, et al. "Linformer: Self-attention with linear complexity." (2020). link.

Transformers - Drawbacks

- Other drawbacks, improvement areas:
 - Positional encoding representations:
 - Do we need absolute indices to represent position?

$$f_{t:t \in \{q,k,v\}}({m{x}}_i,i) := {m{W}}_{t:t \in \{q,k,v\}}({m{x}}_i + {m{p}}_i)$$

- Slew of works and variants has been proposed to the vanilla (sinusoidal, absolute) position encoding we saw
- General trend:
 - Move towards relative position encoding
 - E.g. Relative linear position attention [Shaw et al. 2018]

 $f_q(\boldsymbol{x}_m) := \boldsymbol{W}_q \boldsymbol{x}_m$ $f_k(\boldsymbol{x}_n, n) := \boldsymbol{W}_k(\boldsymbol{x}_n + \tilde{\boldsymbol{p}}_r^k)$ $f_v(\boldsymbol{x}_n, n) := \boldsymbol{W}_v(\boldsymbol{x}_n + \tilde{\boldsymbol{p}}_r^v)$ Relative distance between pos. m and n $r = clip(m - n, r_{min}, r_{max})$

where $ilde{m{p}}_r^k, ilde{m{p}}_r^v \in \mathbb{R}^d$ are trainable relative position embeddings

[Aside] Rotary Position Embeddings

- RoPE now adopted default in modern LLMs
 - Encodes absolution position with a rotation matrix
 - RoPE + Transformer = RoFormer

Model	BLEU
Transformer-baseVaswani et al. [2017]	27.3
RoFormer	27.5

Table 2: Comparing RoFormer and BERT by fine tuning on downstream GLEU tasks.

Model	MRPC	SST-2	QNLI	STS-B	QQP	MNLI(m/mm)
BERTDevlin et al. [2019]	88.9	93.5	90.5	85.8	71.2	84.6/83.4
RoFormer	89.5	90.7	88.0	87.0	86.4	80.2/79.8

[1] RoPE: Su, Jianlin, et al. "Roformer: Enhanced transformer with rotary position embedding." (2021) [arxiv]

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37

[Aside] GEMM-Based Architecture

Foundation Models Scaling in Model Size and Context

					Claude (2001
00000					
50000					GPT-4 (128K
				Cla	ude (100K)
00000					
50000	GPT-2 (1K)			GF	PT-4 (32K)
GPT-1 (512)	GPT-3	(2K)	GPT-3.	5 (4K) 🔎
0 📥	-				
	January 2019	January 2020	January 2021	January 2022	January 2023
			Year		

Scaling in Model Size: 100M to 500B in Four Years

Scaling in Sequence Length: 512 to 200K in Five Years

Our Current Models Scale Quadratically

Quadratic scaling in sequence length N, model dimension d

Can we Scale Sub-Quadratically?

Can we find a single primitive that scales sub-quadratically to replace both?

Slide credits with thanks to: Daniel Fu <danfu@cs.standford.edu>

[Aside] GEMM-Based Architecture

Yes... The Key is Monarch Matrices!

Artistic Rendition of "Monarch Mixer" (DALL-E 3)

Monarch Mixer (M2): new sub-quadratic, hardware-efficient architecture

- Scales **sub-quadratically** in context length, model dimension
- Matches BERT, ViT quality with up to 50% fewer FLOPs, **faster wall-clock**
- M2-BERT for long-document retrieval

Gated Convolutions: A Match for Attention?

Monarch Mixer: Sub-Quadratic Mixing for Both

y GeLU/ReLU GeLU/ReLU

Slide credits with thanks to: Daniel Fu <danfu@cs.standford.edu>

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39

TRANSFORMER BASED LANGUAGE MODELS

Architectural Variants

- The Transformers architecture underpins most SoTA LLMs of today.
- There are 3 main variations of the encoderdecoder blocks we studies for Transformers in L6
 - Encoders e.g. models: **BERT** and BERT-variants
 - Decoders e.g. the **GPT** series
 - Encoder-Decoder e.g. vanilla transformer, T5, Flan-T5^[1] (instruction tuned T5) etc.

[1] Flan-T5 - Chung, Hyung Won, et al. "Scaling instruction-finetuned language models.". link.

	Ranl	< Name	Model	URL	Score	CoLAS	SST-2	MRPC	STS-B	QQP	
	1	T5 Team - Google	Т5		89.7	70.8	97.1	91.9/89.2	92.5/92.1	74.6/90.4	
	2	ALBERT-Team Google Languag	JeALBERT (Ensemble)		89.4	69.1	97.1	93.4/91.2	92.5/92.0	74.2/90.5	BERT
+	3	王玮	ALICE v2 large ensemble (Alibaba DAMO NLP)		89.0	69.2	97.1	93.6/91.5	92.7/92.3	74.4/90.7	N
	4	Microsoft D365 AI & UMD	FreeLB-RoBERTa (ensemble)		88.8	68.0	96.8	93.1/90.8	92.4/92.2	74.8/90.3	
	5	Facebook Al	RoBERTa		88.5	67.8	96.7	92.3/89.8	92.2/91.9	74.3/90.2	
	6	XLNet Team	XLNet-Large (ensemble)		88.4	67.8	96.8	93.0/90.7	91.6/91.1	74.2/90.3	
+	7	Microsoft D365 AI & MSR AI	MT-DNN-ensemble		87.6	68.4	96.5	92.7/90.3	91.1/90.7	73.7/89.9	
	8	GLUE Human Baselines	GLUE Human Baselines		87.1	66.4	97.8	86.3/80.8	92.7/92.6	59.5/80.4	Humans
	9	Stanford Hazy Research	Snorkel MeTaL		83.2	63.8	96.2	91.5/88.5	90.1/89.7	73.1/89.9	N
	10	XLM Systems	XLM (English only)		83.1	62.9	95.6	90.7/87.1	88.8/88.2	73.2/89.8	

• The age of humans is over?

Think of the encoder part of the transformer architecture

- Landmark, pivotal neural LM that has become an ubiquitous baseline in NLP.
- BERT is conceptually simple (multi-layer, bidirectional transformer), empirically powerful.

 Unlike predecessors (ELMo) or contemporaneous LMs (GPT), BERT is deeply bidirectional and independent of task-specific features with unified architecture across different tasks.

Devlin et al. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. (2019). [arxiv]

Code and models: https://github.com/google-research/bert [Colab]

Google Al

43

- First, pre-trained on (large) unlabeled data on two unsupervised tasks/objectives:
 - Masked LM (MLM), and
 - Next Sentence Prediction (NSP)
- Then, fine-tuned using labeled data from downstream tasks
- Training entails feeding the final hidden vectors to an output linear layer with softmax over the possibilities (e.g. the vocabulary as in a standard LM)

Devlin *et al.* BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. (2019). [arxiv] Code and models: <u>https://github.com/google-research/bert</u> [Colab] **Google A**

Pre-training objectives

```
Input: The man went to the [MASK]<sub>1</sub> . He bought a [MASK]<sub>2</sub> of milk .
Labels: [MASK]<sub>1</sub> = store; [MASK]<sub>2</sub> = gallon
```

- 80% of the target words are masked with: [MASK]. 10% are replaced with another word, and 10% are kept as-is, to bias 'towards the observation'.
- *Variants*: masking granularity can be varied (word-piece, word, span) with respective quirks. E.g., masking named entities improves structured knowledge representation.
- Next sentence prediction (NSP): does sentence B follow A?

- 50% of the time true, 50% of the time it's a random sentence.
- Later research finds removing the NSP task does not hurt, or slightly improves performance. ^[2]

Aroca-Ouellette S, Rudzicz F (2020) <u>On Losses for Modern Language Models</u>, EMNLP.
 Rogers, Anna et al. "A primer in BERTology: What we know about how BERT works." TACL(2020). <u>link</u>

Findings from ablative studies ^[1,2,3]

• **Heads**: Analysis of the multi-headed attention mechanism in BERT shows attention heads exhibiting attentions on various linguistic (e.g. syntax, coreference) patterns. ^[1]

- Layers: linear word order and surface features captured most by lower layers. Syntactic information most prominent in middle layers. Semantic and task specific features are best captured in higher/final layers.
- Research on proposed improvements and modifications to BERT, both architectural choices (e.g. # of layers, heads) and training methods is voluminous and ongoing. Due to overall trend towards larger model sizes, systematic ablations have become prohibitively expensive.

^{1.} Clark et al. "What does bert look at? an analysis of bert's attention." (2019). link

^{2.} Tenney et al. "BERT rediscovers the classical NLP pipeline." (2019). link

^{3.} Rogers, Anna et al. "A primer in BERTology: What we know about how bert works." TACL(2020). link

Findings from ablative studies

- Limitations: BERT's possession of impressive syntactic, semantic, and world knowledge has caveats.
- World Knowledge:
 - BERT struggles with pragmatic inference, and role-based event knowledge.
 - It can 'guess' object affordances and properties but cannot reason about relationships between them. Example: it 'knows' people can walk into houses, houses are big, but cannot infer that houses are bigger than people.

• Semantic Knowledge:

- Struggles with representations of numbers.
- Surprisingly brittle to *named entity* replacements: e.g. 85% drop in performance in coreference task with names replaced.

• Syntactic Knowledge:

- Does not 'understand' negations and is insensitive to malformed input.
- Findings suggest that either its syntactic knowledge is incomplete, or not dependent on it for solving its tasks.

Why BERT matters/mattered?

System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	Average
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
BERTBASE	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
BERTLARGE	86.7/85.9	72.1	92.7	94.9	60.5	86.5	89.3	70.1	82.1

System	Dev	Test
ESIM+GloVe	51.9	52.7
ESIM+ELMo	59.1	59.2
OpenAI GPT	-	78.0
BERTBASE	81.6	-
BERTLARGE	86.6	86.3
Human (expert) [†]	-	85.0
Human (5 annotations) [†]	-	88.0

system	<i>D</i>	ev	Test		
	EM	F1	EM	F1	
Top Leaderboard System	s (Dec	10th,	2018)		
Human			82.3	91.2	
#1 Ensemble - nlnet	-	-	86.0	91.7	
#2 Ensemble - QANet	-	-	84.5	90.5	
Publishe	d				
BiDAF+ELMo (Single)	-	85.6	-	85.8	
R.M. Reader (Ensemble)	81.2	87.9	82.3	88.5	
Ours					
BERT _{BASE} (Single)	80.8	88.5	-	-	
BERTLARGE (Single)	84.1	90.9	-	-	
BERTLARGE (Ensemble)	85.8	91.8		-	
BERTLARGE (Sgl.+TriviaQA)	84.2	91.1	85.1	91.8	
BERTLARGE (Ens.+TriviaQA)	86.2	92.2	87.4	93.2	

Dav

Suctors

- Performance and versatility:
 - Impressive performance not only beating (then) SOTA peers, but humans too!
 - Popularized the pipeline of 'pretraining' -> 'fine-tuning' NLMs
 - Fine-tuning (pre-trained) BERT on downstream tasks led to new SOTA results on a broad range of NLP tasks

Use BERT for everything?

- BERT has an encoder-only architecture
- While the preceding results are great, but pretrained encoders aren't great for everything
- For example, tasks involving generating sequences auto-regressively (one token at a time) - like our machine translation task!
- Solution: use a (pretrained) decoder in conjunction

Aside – BERT → BART → NMT

- Explosion of variants to BERT
- Pretrained BERT language model used to re-score/fine-tune downstream NLP tasks
- BART (Lewis *et al*, 2020) adds the decoder back to BERT, keeping the BERT objective
- Add some source language layers on top to train for NMT

Lewis, Mike, et al. "Bart: Denoising sequence-to-sequence pre-training for natural language generation, translation, and comprehension." (2019). <u>link</u>.

T5: Text-to-Text Transfer Transformer

A *refined* Transformer updated with better methodologies

- T5 is an unified framework that casts all NLP problems into a 'text-to-text' format.
- Architecturally (almost) identical to the original Transformer (Vaswani et al., 2017).
- Draws from a systematic study comparing pre-training objectives, architectures, unlabeled data sets, transfer approaches, and other factors on dozens of language understanding tasks.
- Introduces and uses a new curated dataset: "Colossal Clean Crawled Corpus" (C4) for training.

Distinguishing features:

- Consistent, task-invariant MLE training objective.
- Self-attention "mask" with prefix.
- Unsupervised "denoising" training objectives: *span corruption* (conceptually same to MLM, mask 'spans' instead of words).

1. Raffel et al. "Exploring the limits of transfer learning with a unified text-to-text transformer." (2020). link

T5: Text-to-Text Transfer Transformer

Example Task: English to German (En-De) translation:

Input sentence: "*That is good*." Target: "*Das ist gut*."

 Training: task specification is imbued by prepending task prefix to the input sequence. Model trained on next sequence prediction over the concatenated input sequence:

"translate En-De: That is good. Das ist gut."

- For prediction, the model is fed **prefix**:
 - "translate En-De: That is good. target:"
- For **classification** tasks, the model predicts a single word corresponding to the target label.
- E.g. MNLI task of entailment prediction:
 - "mnli premise: I hate pigeons. hypothesis: I am hostile to pigeons. entailment."
- Model predicts label: {"entailment", "neutral", "contradiction"}.

Input/Output format for training denoising objective

T5: Text-to-Text Transfer Transformer

Why T5 matters?

- Unifying diverse NLP problems as one ('*text-to-text*') format is a **really cool idea**.
- This allows us to use the same model, loss function, hyperparameters etc. across a diverse set of tasks

 Remarkable transfer learning capabilities: T5 can be finetuned to answer a wide range of (open-domain dataset NQ, WQ, TQA) questions, retrieving knowledge from its parameters

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On that note – A2 BART Analysis

- **Code Demo** HuggingFace [t5_small|BART-base] NMT trained on Hansard (Fr-En)
- https://huggingface.co/docs/transformers/model_doc/bart
- https://huggingface.co/raeidsaqur/bart-base
- https://huggingface.co/raeidsaqur/mt_fr2en_hansard_t5-small
- Optional: bonus pointers

Lewis, Mike, et al. "Bart: Denoising sequence-to-sequence pre-training for natural language generation, translation, and comprehension." (2019). <u>link</u>.

GPT SERIES

GPT: Generative Pretrained Transformers

Open AI GPT-series of models – uses multi-layer decoder only blocks

• Open AI GPT papers: GPT (2018)^[1], GPT-2 (2019)^[2], GPT-3 (2020)^[3]

- Architecturally (almost) identical each scales (params, data) on predecessor
- Pretraining objective is classic 'language modeling', to maximize the likelihood:
- Specifically, given an unsupervised corpus of tokens μ = {μ₁, ..., μ_n}, where k is context window, P is modelled using a neural network with parameters θ.

$$p(x) = \prod_{i=1}^{n} p(s_n | s_1, ..., s_{n-1})$$

$$L_1(\mathcal{U}) = \sum_i \log P(u_i | u_{i-k}, \dots, u_{i-1}; \Theta)$$

- 1. Radford, Alec, et al. "Improving language understanding by generative pre-training." (2018)
- 2. Radford, Alec, et al. "Language models are unsupervised multitask learners." OpenAI Blog 1.8 (2019)
- 3. Brown, Tom B., et al. "Language models are few-shot learners." arXiv preprint arXiv:2005.14165 (2020)

GPT: Generative Pretrained Transformers

- Distinguishing features:
 - Uses multi-layer transformer **decoder only blocks**
 - Auto-regressive generative model, does not see the future (no bidirectional awareness)
 - Like traditional LMs, outputs one token at a time

- 1. Radford, Alec, et al. "Improving language understanding by generative pre-training." (2018)
- 2. Radford, Alec, et al. "Language models are unsupervised multitask learners." OpenAl Blog 1.8 (2019)
- 3. Brown, Tom B., et al. "Language models are few-shot learners." arXiv preprint arXiv:2005.14165 (2020)

Key architectural differences

- GPT vs. BERT-variants:
 - GPT uses 'transformer' blocks as *decoders*, and BERT as *encoders*.
 - Underlying (block level) ideology is same
 - GPT (later Transformer XL, XLNet) is an **autoregressive** model, BERT is not
 - At the cost of auto-regression, BERT has bi-directional context awareness.
 - GPT, like traditional LMs, outputs (predicts) one token at a time.
- Compare with T5, BART that uses encoder-decoder

[1] Radford, Alec, et al. "Improving language understanding by generative pre-training." (2018).

GPT-3 LLMs take off ...

- Increasingly convincing results permeating into the public sphere and zeitgeist
- In-context learning:

Figure 1.1: Language model meta-learning. During unsupervised pre-training, a language model develops a broad set of skills and pattern recognition abilities. It then uses these abilities at inference time to rapidly adapt to or recognize the desired task. We use the term "in-context learning" to describe the inner loop of this process, which occurs within

1. Brown, Tom B., et al. "Language models are few-shot learners." arXiv preprint arXiv:2005.14165 (2020)

GPT-3: In context learning + ... prompting

The notion of 'prompting' begins to emerge ... ullet

The	three settings we explore for in-	context learning	Traditional	fine-tuning (not
Zero	-shot		Fine-tuning	
The desc	model predicts the answer given only a ription of the task. No gradient updates	natural language are performed.	The model is large corpus	trained via repeated of example tasks.
	Translate English to French:	← task description	1 sea ot	ter => loutre de
	cheese =>	← prompt		\mathbf{V}
				\checkmark
One	shot		1 pepper	mint => menthe p
in ac	ldition to the task description, the mode	l sees a single		\checkmark
exar	nple of the task. No gradient updates ar	e performed.		
	Translate English to Erench:	← task description		\checkmark
	and ottor => loutro do mor	evemple		↓
		example	1 plush	giraffe => girafe
	cheese =>	← prompt		
				gradient update
Fow	ehot			
In ac	Idition to the task description, the mode	l sees a few	1 cheese	=>
exar	nples of the task. No gradient updates a	re performed.		
	Translate English to French:	← task description		
	sea otter => loutre de mer	← examples		
	<pre>peppermint => menthe poivrée</pre>	\leftarrow		
	<pre>plush girafe => girafe peluche</pre>	<i>←</i>		
	cheese =>	← prompt		

used for GPT-3)

gradient updates using a

prompt

Figure 2.1: Zero-shot, one-shot and few-shot, contrasted with traditional fine-tuning. The panels above show

GPT-3: In context learning + ... prompting

• The notion of 'prompting' begins to emerge ...

Figure 1.2: Larger models make increasingly efficient use of in-context information. We show in-context learning

GPT-3: Models

- Initialization, pre-normalization (inherited from GPT2).
- 8 model sizes trained to study effect of model size

Model Name	$n_{\rm params}$	$n_{\rm layers}$	$d_{\rm model}$	$n_{\rm heads}$	$d_{\rm head}$	Batch Size	Learning Rate
GPT-3 Small	125M	12	768	12	64	0.5M	$6.0 imes 10^{-4}$
GPT-3 Medium	350M	24	1024	16	64	0.5M	$3.0 imes 10^{-4}$
GPT-3 Large	760M	24	1536	16	96	0.5M	$2.5 imes 10^{-4}$
GPT-3 XL	1.3B	24	2048	24	128	1M	$2.0 imes 10^{-4}$
GPT-3 2.7B	2.7B	32	2560	32	80	1M	$1.6 imes 10^{-4}$
GPT-3 6.7B	6.7B	32	4096	32	128	2M	$1.2 imes 10^{-4}$
GPT-3 13B	13.0B	40	5140	40	128	2M	$1.0 imes 10^{-4}$
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128	3.2M	$0.6 imes 10^{-4}$

Table 2.1: Sizes, architectures, and learning hyper-parameters (batch size in tokens and learning rate) of the models which we trained. All models were trained for a total of 300 billion tokens.

GPT-3: Training Datasets

- Datasets
 - Common Crawl dataset: nearly a trillion words, with quality curation.
 - Added: WebText, Books1, 2 and English Wikipedia

Train time

Dataset	Quantity (tokens)	Weight in training mix
Common Crawl (filtered)	410 billion	60%
WebText2	19 billion	22%
Books1	12 billion	8%
Books2	55 billion	8%
Wikipedia	3 billion	3%

GPT-3: Results

- TL;DR: unprecedently impressive results across task domains
 - Performance (e.g. world knowledge) increases with size
- Datasets grouped to 9 categories of downstream tasks
 - Examples: language modeling, QA, translation, Winograd, common-sense reasoning, reading comprehension, NLI etc.
 - Read the paper for details

Setting	PTB	
SOTA (Zero-Shot)	35.8 ^a	
GPT-3 Zero-Shot	20.5	

Table 3.1: Zero-shot results on PTB language modeling dataset. Many other common language modeling datasets are omitted because they are derived from Wikipedia or other sources which are included in GPT-3's training data. ^{*a*}[RWC⁺19]

Setting	LAMBADA (acc)	LAMBADA (ppl)	StoryCloze (acc)	HellaSwag (acc)
SOTA	68.0^{a}	8.63 ^b	91.8 ^c	85.6 ^d
GPT-3 Zero-Shot	76.2	3.00	83.2	78.9
GPT-3 One-Shot	72.5	3.35	84.7	78.1
GPT-3 Few-Shot	86.4	1.92	87.7	79.3

Table 3.2: Performance on cloze and completion tasks. GPT-3 significantly improves SOTA on LAMBADA while achieving respectable performance on two difficult completion prediction datasets. *a*[Tur20] *b*[RWC⁺19] *c*[LDL19] *d*[LCH⁺20]

Figure 3.3: On TriviaQA GPT3's performance grows smoothly with model size, suggesting that language models continue to absorb knowledge as their capacity increases. One-shot and few-shot performance make significant gains over zero-shot behavior, matching and exceeding the performance of the SOTA fine-tuned open-domain model, RAG $[LPP^+20]$

DIFFERENT DIRECTIONS

Token free models

- Unlike the ubiquitous pre-trained LMs that operate on sequences of tokens corresponding to word or sub-word units, token free models:
 - Operate on raw text (bytes or characters) directly.
 - Removes necessity for (error-prone, complex) text preprocessing pipelines.
 - Con: raw sequences significantly longer than token sequences, increases computational complexity. (Reminder: 'attention' costs are quadratic to the length of input sequence)

Clark et al. "CANINE: Pre-training an efficient tokenization-free encoder for language representation." (2021). <u>link</u>
 Xue et al. "ByT5: Towards a token-free future with pre-trained byte-to-byte models." (2022). <u>link</u>

Token free models

- Pitfalls of explicit (word, sub-word) tokenization:
 - Need for large language dependent (fixed) vocabulary mapping matrices.
 - Applies hand-engineered, costly, language-specific string tokenization/segmentation algorithms (e.g. BPE, word-piece, sentence-piece) requiring linguistic expertise.
 - Heuristic string-splitting, however nuanced, cannot capture full breadth of linguistic phenomena, (e.g. morphologically distant agglutinative, non-concatenative languages). Other examples include languages without white-space (Thai, Chinese), or that uses punctuation as letters (Hawaiian, Twi). *Fine-tuning* tokenization needs to match *pretraining* tokenization methods.
 - Brittle to noise, corruption of input (typos, adversarial manipulations). Corrupted tokens lose vocabulary coverage.

Clark et al. "CANINE: Pre-training an efficient tokenization-free encoder for language representation." (2021). <u>link</u>
 Xue et al. "ByT5: Towards a token-free future with pre-trained byte-to-byte models." (2022). <u>link</u>

[Aside] Token free models - CANINE

CANINE: Character Architecture with No tokenization In Neural Encoders.

- CANINE is a large language encoder with a deep transformer stack at its core.
- Inputs to the model are sequences of Unicode characters. 143,698 Unicode codepoints assigned to characters covers 154 scripts and over 900 languages!
- To avoid slowdown from increasing sequence length, it uses **stride convolutions to down-sample** input sequences to a shorter length, before the deep transformer stack to encode context.
- Three primary components:
 - Vocab free embedding technique;
 - Character-level model (CLM) with efficiency measures (up/down sampling of sequences); and
 - Perform **unsupervised** masked LM (MLM) pretraining on the CLM using variants:
 - Autoregressive character prediction
 - Subword prediction

Clark et al. "**CANINE**: Pre-training an efficient tokenization-free encoder for language representation." (2022).

[Aside] Token free models - CANINE

• The overall functional composition form uses [UP|DOWN]-sampling, and primary encoder:

 $Y_{seq} \leftarrow UP(ENCODE(DOWN(e)))$ where $e \in \mathbb{R}^{n \times d}$ is an input characters sequence, and $Y_{seq} \in \mathbb{R}^{n \times d}$ is output of sequence predictions

• **Down-sampling**: $h_{init} \leftarrow \text{LOCALTRANSFORMER}(e)$; $h_{down} \leftarrow \text{STRIDEDCONV}(h_{init}, r)$

where $h_{down} \in \mathbb{R}^{m \times d}$ and $m = \frac{n}{r}$ is the number of downsampled positions

• Up-sampling: prediction require model's output layer sequence length to match input's length

 $h_{up} \leftarrow \text{CONV}(h_{init} \oplus h'_{down}, w); \quad y_{seq} \leftarrow \text{TRANSFORMER}(h_{up})$

where \oplus is vector concatenation, CONV projects $\mathbb{R}^{n \times 2d}$ back to $\mathbb{R}^{n \times d}$ across a window of w characters. Applying a final transformer layer yields a final sequence representation: $Y_{seq} \in \mathbb{R}^{n \times d}$

