### Vaswani et al. (2017) still being state of the art





Dr. Vaswani or: How I learned to stop using LSTMs and Love Attention \*obligatory Michael Bay Transformer\*



Vaswani et al. 2017



Vaswani et al. (2017) still being state of the art



UBC Machine Learning Reading Group – Fall 2022 Alan Milligan alanmil@student.ubc.ca



me after making slides!

Not this Vaswani





DISCLAIMER: I am not really a deep learning person and definitely not an NLP person, so I might (read will) make some errors > 90% of these slides were made in the last 24 hours so they also probably have issues



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Not this Vaswan





### We live in the age of transformers

1 of 93 matches Begins with 😌 🔍 transformer

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#### Attention is all you need

Advances in Neural Information Processing Systems 34 (NeurIPS 2021)

NeurIPS Proceedings 🔿 🕩

<u>A Vaswani, N Shazeer, N Parmar</u>... - Advances in neural ..., 2017 - proceedings.neurips.cc ... the number of **attention** heads and the **attention** key and value dimensions, keeping the amount of computation constant, as described in Section 3.2.2. While single-head **attention** is 0.9 ...  $\therefore$  Save  $\overline{99}$  Cite Cited by 53265 Related articles All 46 versions  $\gg$ 

- In the way AlexNet and CNNs revolution computer vision, the advent of the transformer has revolutionized NLP (and several other fields)
- GPT-*x*, BERT, AlphaFold2, SWITCH-C, CLIP,
   DALL-E and many other famous models
   are all based on transformers
- If you want publications and have big (like really big) computers, you may want to consider training giant transformers





### We live in the age of transformers

#### Attention is all you need

<u>A Vaswani</u>, <u>N Shazeer</u>, <u>N Parmar</u>... - Advances in neural ..., 2017 - proceedings.neurips.cc ... the number of **attention** heads and the **attention** key and value dimensions, keeping the amount of computation constant, as described in Section 3.2.2. While single-head **attention** is 0.9 ... - In the way AlexNet and CNNs revolution computer vision, the advent of the transformer has revolutionized NLP (and

### TLDR: All those fancy models by Google/OpenAI/Deepmind/Meta are often just really big transformers

		1 of 67 matches Begins with 🕤 🔍 transformer 🔇
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If you want publications and have big (like really big) computers, you may want to consider training giant transformers.



### Suppose Fred and I go to his favourite German restaurant and I want to look (sound?) cool

### "A blast from the past"

### **Rule Based Methods**

- We can try to hard code language rules
- This incorporates lots of domain knowledge from the source and target language
- These were the original methods developed in the 1970s

Machine Translation



### Statistical Methods

- We look at frequencies across large corpora
- Modeling probabilities of translated phrases conditioned on original phrases
- Used things like Hidden Markov Models and context free grammars, much closer to "machine learning" and used in the mid 2000s

$$ilde{e} = arg \max_{e \in e^*} p(e|f) = arg \max_{e \in e^*} p(f|e) p(e).$$



### Suppose Fred and I go to his favourite German restaurant and I want to look (sound?) cool

### I speak zero German but $\epsilon$ French so I will use this example

"I like the green cat."

How can we go about translating this (simple) sentence?



"J'aime le chat vert."







> Atte

tention





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#### Suppose Fred and I go to his favourite German restaurant and I want to look (sound?) cool

#### "I like the green cat."



CHINESE (SIMPLIFIED) - DETECTED ENGLISH SPANISH FRENCH ✓	← ENGLISH SPANISH ARABIC ∨
《施氏食狮史》 × 石室诗土施氏,嗜狮,誓食十狮。 氏时时适市视狮。 十时,适十狮适市。 是时,适施氏适市。 氏视是十狮,恃矢势,使是十狮逝世。 氏拾是十狮尸,适石室。 石室湿,氏使侍拭石室。 石室拭,氏始试食是十狮。 食时,始识是十狮尸,实十石狮尸。 试释是事。	<ul> <li>"History of Shi's Lion Eating"</li> <li>Shishi Shishi, a poet in the stone room, was addicted to lions and swore to eat ten lions.</li> <li>It is always appropriate to see the lion in the city.</li> <li>At ten o'clock, the ten lions are suitable for the city.</li> <li>It's time for Shishi's market.</li> <li>Shi regarded the ten lions as ten lions.</li> <li>Shi Shi is ten lion corpses, suitable for stone chambers.</li> <li>The stone room was wet, so the clergyman wiped the stone room.</li> <li>The stone room was wiped, and Shi Shi began to try to eat ten lions.</li> <li>When eating, Shi Shi was ten lion corpses, in fact ten stone lion</li> </ul>
"Shī shì shíshī shi" shíshì shī shì shī shì, shì shī, shì shíshí shí. Shì shí shíshìshì shì shī. Sh	corpses. Explanation is a thing.

Good rule based or statistical models could probably handle this fine but things get harder...

Oh hey it's the mid 2010s and deep learning just happened! What can we do!





- Suppose there exists some continuous space of "meaning", where every sentence in every language is represented the same
- Could we build a function that takes a language into meaning land?

Machine Translation

LSTMs





### How do we make sentences continuous?

### "I like the green cat."



["I", "like", "the", "green", "cat", "."]

[23, 796, 4012, 8923, 4850, 42]



[-2.03, 0.799, 0.448, 1.34, 1.14, -0.039], [-1.71, -0.163, 0.863, -1.01, 1.21, 0.73], [-0.932, -0.599, 0.558, -1.13, 1.54, 1.34], [0.782, -0.542, -0.00264, -0.99, -1.9, 0.399]

Machine Translation

#### Tokenization

- A sentence is broken up into "tokens"
- These could be words, word parts, or characters
- There also special tokens like "<SOS>", "<EOS>", "<OOV>", and "<PAD>"

### Convert to token IDs

- Each token is assigned an ID from a predefined lookup table
- You could think of this like a one hot vector but its usually a dictionary

### Token Embedding

- Each token ID is assigned a vector in a fixed dimension (512 in Vaswani)
- These vectors are initialized with Gaussian noise
- Over the course of training, the embedding vector is treated as a parameter and gradients are propagated into the vector to train



### Warning: Entering hand wavey zone





"I think you should be more explicit here in step two."



How about we have a neural network eat these vectors one by one, plus the output of the previous step



 $x_t$  = source embedding vectors  $h_t$  = latent state vectors  $y_t$  = predicted token f = neural network

#### PROBLEMS:

- It's hard to model long range dependencies because the model sees  $x_n$  much later than  $x_0$
- $h_{encoding}$  is of fixed size, so it can only hold so much information (related to the first point)
- Optimization is hard because propagating gradients backwards in time involves taking matrices to high powers, leading to vanishing or exploding gradient

Visually, (using some Stanford guy's notation)



# Recurrent Neural Network TLDR

How about we have a neural network eat these vectors one by one, plus the output of the previous step



Note: I am skipping a lot of details like what the inside of that neural network actually looks like, but hopefully this gives an intuition



model sees  $x_n$  much later than  $x_0$ 

- *h*<sub>encoding</sub> is of fixed size, so it can only hold so much information (related to the first point)
- Optimization is hard because propagating gradients backwards in time involves taking matrices to high powers, leading to vanishing or exploding gradient

### Long Short-Term Memory TLDR ("fancy" RNNs)

Instead of just storing  $h_t$  as a function of  $x_t$  and  $h_{t-1}$ , we can also store another hidden state  $c_t$ 

### Possibly Flawed Intuition

-

-

- Let  $h_t$  be the "short term memory," updated by a network output of each new input and previous short-term memory
- Let  $c_t$  be the "long term memory," updated by a learned linear combination of previous memory and the input

#### Unreadable Math

$$egin{aligned} f_t &= \sigma_g(W_f x_t + U_f h_{t-1} + b_f) ext{(forget)} \ i_t &= \sigma_g(W_i x_t + U_i h_{t-1} + b_i) \ ext{(input)} \ o_t &= \sigma_g(W_o x_t + U_o h_{t-1} + b_o) \ ext{(output)} \ ilde{c}_t &= \sigma_c(W_c x_t + U_c h_{t-1} + b_c) \ ext{(candidate memory)} \ c_t &= f_t \odot c_{t-1} + i_t \odot ilde{c}_t \ ext{(updated long memory)} \ h_t &= o_t \odot \sigma_h(c_t) \ \end{aligned}$$



### Benefits

Long term memory acts like residual connections which allow for much better gradient flow during optimization

LSTMs

(ideally) the network can learn to remember important stuff in  $c_t$ 

Machine Translation

### Remaining Issues

- The amount of information that can be propagated forward is still fixed and long term dependencies can still be forgotten
- Vanishing/Exploding gradient can still happen albeit less

### Long Short-Term Memory TLDR ("fancy" RNNs)

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#### Unreadable Math

 $f_t = \sigma_g(W_f x_t + U_f h_{t-1} + b_f)$  (forget) $i_t = \sigma_g(W_i x_t + U_i h_{t-1} + b_i)$  (input)



### Note: I am skipping a lot of details again

#### Benefits

- Long term memory acts like residual connections which allow for much better gradient flow during optimization
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Machine Translation

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### Summary: RNNs are problematic







### Summary: RNNs are problematic















### Finally, pay Attention (in an RNN)

**LSTMs** 

How can we better model long range dependencies?

Idea: In the decoding phase, use a weighted combination of all  $h_t$  so that we "pay attention" to the more important parts of the  $h_t$ 



### Step 1

Generate all  $h_t$  in the encoding phase

Step 2

Repeat for until <EOS> token



Compute Score( $s_i$ ,  $h_j$ ) for current decoder state  $s_i$  and all encoder states  $h_j$ 

Step 2.2

Compute attention weights as Softmax(scores)



### Step 3

Profit

Attention

Machine Translation



Sounds reasonable, but in order to compute the attention weights, we need some sort of scoring function

Options from Lilian Weng's blog			
Name	Alignment score function	Citation	
Content-base attention	$ ext{score}(oldsymbol{s}_t,oldsymbol{h}_i) =  ext{cosine}[oldsymbol{s}_t,oldsymbol{h}_i]$	Graves2014	
Additive(*)	$ ext{score}(oldsymbol{s}_t,oldsymbol{h}_i) = \mathbf{v}_a^ op  anh(\mathbf{W}_a[oldsymbol{s}_t;oldsymbol{h}_i])$	Bahdanau2015	
Location-Base	$ \begin{aligned} &\alpha_{t,i} = \mathrm{softmax}(\mathbf{W}_a \boldsymbol{s}_t) \\ &\text{Note: This simplifies the softmax alignment to only depend on the target position.} \end{aligned} $	Luong2015	
General	$ ext{score}(m{s}_t,m{h}_i) = m{s}_t^\top \mathbf{W}_a m{h}_i$ where $\mathbf{W}_a$ is a trainable weight matrix in the attention layer.	Luong2015	
Dot-Product	$ ext{score}(oldsymbol{s}_t,oldsymbol{h}_i)=oldsymbol{s}_t^{ op}oldsymbol{h}_i$	Luong2015	
Scaled Dot-Product(^)	$\operatorname{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \frac{\boldsymbol{s}_t^{\top} \boldsymbol{h}_i}{\sqrt{n}}$ Note: very similar to the dot-product attention except for a scaling factor; where n is the dimension of the source hidden state.	Vaswani2017	

**LSTMs** 

Some authors use score functions with learned parameters

We focus on scaled dot-product attention as it is used in Vaswani et al.

$$ext{score}(oldsymbol{s}_t,oldsymbol{h}_i) = rac{oldsymbol{s}_t^ opoldsymbol{h}_i}{\sqrt{n}}$$

Recall from math that a dot product is a measure of similarity in a vector space

Attention

Machine Translation



Sounds reasonable, but in order to compute the attention weights, we need some sort of scoring function

	Options from Lilian Weng's blog	7	
Name Alignment score function		Citation	Some authors use score functions with learned
Contont_br	0.026		parameters

### TLDR: Attention is a method of deciding which inputs to care about

Dot-Product	$ ext{score}(oldsymbol{s}_t,oldsymbol{h}_i)=oldsymbol{s}_t^{ op}oldsymbol{h}_i$	Luong2015
Scaled Dot-Product(^)	score $(s_t, h_i) = \frac{s_t^{T} h_i}{\sqrt{n}}$ Note: very similar to the dot-product attention except for a scaling factor; where n is the dimension of the source hidden state.	Vaswani2017

in Vaswani et al.

$$ext{score}(oldsymbol{s}_t,oldsymbol{h}_i) = rac{oldsymbol{s}_t^ opoldsymbol{h}_i}{\sqrt{n}}$$

Recall from math that a dot product is a measure of similarity in a vector space

Machine Translation



### Enter Michael Bay: The Transformer

#### In an RNN with attention we are using all $h_t$ , why don't we just ditch the recurrent part



Vaswani et al. proposes: "Attention is all you need"

- Have an encoder where all input embeddings pay attention to all other input embeddings
- Add "positional encodings" to input embeddings so that the sequential structure is retained
- Have a decoder that pays attention to all input embeddings as well as the already decoded embeddings

Transformers

Attention



### Step 1: Self-Attention Encoder

**LSTMs** 

Lets build a Transformer Encoder!



**Machine Translation** 

### Encoder Objective

Create an "interesting" learned representation of the inputs useful for the Decoder (next)

#### Ingredients

- 1. Embeddings + Positional Encodings
- 2. Multi-Head Attention
- 3. Residual Connection and Layer Norm

Attention

Transformers

4. Fully Connected Layer



### Word Embedding

Same as earlier, Token IDs mapped into real vectors that are learned during training

### **Positional Encoding**

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{model}})$$
  
 $PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{model}})$ 



- Vectors defined by this formula are added to each word embedding vector to add "relative position" between embeddings
- Not intuitive to me, but this formula allows for easy relative position learning via some trigonometric addition identities
- You can also just add torch.nn.Embedding style absolute positional encodings in the same way as word embedding and learn via backpropagation (Vaswani et al. tested this with similar results)

Attention



-

### Step 1.2: Multi-Head Self-Attention

**LSTMs** 

### Here is where the real magic happens

### **Recall Scaled Dot-Product Attention**

$$ext{score}(oldsymbol{s}_t,oldsymbol{h}_i) = rac{oldsymbol{s}_t^{ op}oldsymbol{h}_i}{\sqrt{n}}$$

Attention
$$(\mathbf{s}_t, \mathbf{h}_i) = \frac{e^{\text{score}(\mathbf{s}_t, \mathbf{h}_i)}}{\sum_{j=1}^n e^{\text{score}(\mathbf{s}_t, \mathbf{h}_j)}}$$

- In Vaswani et al, we do a learned projection of the input to produce matrices *Q*, *K*, which are analogous to *s*, *h* above
  - The columns of the non-linear matrix product are akin to the attention weights in the RNN example, we use these weights on another learned projection of the input V

$$\operatorname{Attention}(Q, K, V) = \operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

Machine Translation

### More is Better

- Rather than doing attention once on the input, lets do it N (= 6) times
  - N different copies of projection matrices are learned, attention is run N times, and then all outputs are projected back to  $d_{model}$

 $\begin{aligned} \text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O \\ \text{where head}_i &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \end{aligned}$ 

- More heads mean different heads can learn different things like grammar and vocabulary

Transformers

- Also ensemble good

Attention



#### Layer Normalization

- Given the activations of a layer, we compute the mean and standard deviation
- We subtract and divide by these values respectively, then multiply and add by learned parameters (so that the identity can be learned as in Batch Norm)

$$\mu^{l} = \frac{1}{H} \sum_{i=1}^{H} a_{i}^{l} \qquad \sigma^{l} = \sqrt{\frac{1}{H} \sum_{i=1}^{H} (a_{i}^{l} - \mu^{l})^{2}}$$
  
LayerNorm $(x) = \frac{\gamma}{\sigma^{l}} (x - \mu^{l}) + \beta$ 

something something "reduce internal covariate shift"

**LSTMs** 

### **Residual Connections**

 As with ResNets from vision, instead of directly transforming the input, we learn a residual, then apply layer norm

### LayerNorm(x + Sublayer(x))

Where Sublayer(x) is either Multi-Head Attention or a feed forward network

- Residual Connections have been shown to make optimization easier in cases where transformations should be close to identity maps

Transformers

Attention



Here we have a simple two layer ReLU network that acts on each embedding individually





### Self-Attention Encoder Assembled!



- With these pieces, we can now create a latent representation of an input sentences where each vector has applied self attention N times across h heads
- In Vaswani et al, N = 6 and h = 8
- The output is a matrix of embedding vectors in  $\mathbb{R}^{n imes d_{model}}$  (n x 512)
- We can now use this in step 2: the Decoder





### Step 2: Masked and Cross Attention Decoder



**Machine Translation** 

#### **Decoder Objective**

Given Encoder("I like the green cat. <EOS>") and Decoder("<SOS> J'aime le chat "), predict "vert".

#### Ingredients

- 1. Embeddings + Positional Encodings [Done]
- 2. Masked Self Attention
- 3. Residual Connection and Layer Norm [Done]

Attention

Transformers

- 4. Encoder-Decoder Cross Attention
- 5. Fully Connected Layer [Done]
- 6. Output Layer

**LSTMs** 



- Vaswani et al. wanted to "preserve [the] auto-regressive property" of the model, meaning that no word should be able to attend to words decoded after it
- This is accomplished with "masking," which essentially sets the score of later entries to zero

Visualizing Legal Attention Connections

This triangular mask represents which position each position can attend to





As math,

 $\operatorname{Softmax}(\frac{QK^T}{\sqrt{d_k}} \odot M)V$ 

Where *M* is the lower triangular matrix on the left

Transformers

Attention



- We want the decoder to be able to use the "interesting" representation learned by the encoder
- This is done by letting the decoder embeddings attend to the keys and values of the Encoder





After N decoder layers, we project up to the dimension of the target vocabulary and softmax for predictions



#### Important Note:

During training/testing, we feed in the whole target sentence shifted by <SOS> since the self attention mask will make it seem like you are doing a one step prediction at every position. This was nonobvious to me.

# We have assembled the full Transformer!

**LSTMs** 



- That was a lot of deep learning jargon that I don't expect everyone to understand
- It took me over 10 attempts to grasp all of this and I still have questions

### Transformer TLDR:

- Embed source words with some learnable vector plus positional encodings
- Run a few rounds of scaled dot product self attention plus a layer normalized feedforward network for your source embeddings

Attention

- Embed known target words (or <SOS>) with some learnable vector plus positional encodings
- Run a few rounds of forward masked self attention, cross attention with the encoded source sentence, layer normalization, and a feedforward network

Transformers

- Project and softmax the output, profit



We now know the architecture, but there are still some training details

#### Regularization

- Despite no mention in the paper, all implementations I've seen use "weight decay," also known as L2 regularization
- Dropout is applied to both attention and feed forward layers as well as the embeddings
- "Label Smoothing" which punishes incorrect softmax outputs slightly less

Machine Translation

#### Loss Function

- Cross Entropy loss is applied between the prediction vector and (smoothed) label vector
- The loss is computed independently for each prediction in a forward pass, recalling that we make several predictions concurrently

Attention

**LSTMs** 

#### Optimizer

Everyone's good friend Adam is used for optimization with the following odd learning rate schedule using 4000 warmup steps (no justification provided)

 $lrate = d_{\text{model}}^{-0.5} \cdot \min(step\_num^{-0.5}, step\_num \cdot warmup\_steps^{-1.5})$ 





### How to inference your transformer



#### Beam Search

- To get the better predictions, Vaswani et al. (and NLP in general) will use *BeamSearch(b)*, a process where we autoregressively predict b copies until all reach <EOS>
- Each beam is ranked by total probability, and we only propagate the top b at any given time (the others die)

<FND:

<END>

In this example b = 2



### Transformer Benefits

#### Long Range Dependency

- Self-attention can model arbitrarily long sequences in constant distance
- This completely removes the issue RNNs face about forgetting the start (or middle for bidirectional) of the sequence
- Below are visualized attention weights during translation

### this is the first book i did i (END] Machine Translation

#### **Computational Efficiency**

- Since we no longer have to process sentences token by token, Transformers are extremely parallelizable and GPU friendly
- Self attention masking means each training sequence of length n gives us n gradients from one forward pass
- Every attention had can be on a on a different machine, every layer can be on a different machine, the encoder and decoder can be on different machines, etc.
- Some argue the true reason transformers perform is simply that we are able to scale them to levels that would be impossible for other methods



Attention



nooooo you can't just scale up pure connectionist models on Internet data without inductive biases and modularization and expect them to learn real-world Knowledge and grammar from form, or arithmetic and logical reasoning and causal inference-that's just memorization and superficial patterncommission with intert and social dynamics and multimodal rebotic embodianet which can foster disentagled learning from guided exploration as Gelf-directed patter expressed in Byssian programs and probabilistic can be desired and expressed with uncertainty, and Learnet efficiently on the memory of the series of the submark and exploration and and the series of the



haha gpus go bitterrr



8				8
Madal	BLEU		Training Cost (FLOPs)	
Model	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0\cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3\cdot 10^{19}$	$1.4\cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6\cdot 10^{18}$	$1.5\cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0\cdot 10^{19}$	$1.2\cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0\cdot10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8\cdot 10^{20}$	$1.1\cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	41.29	$7.7\cdot 10^{19}$	$1.2\cdot 10^{21}$
Transformer (base model)	27.3	38.1	$3.3\cdot10^{18}$	
Transformer (big)	28.4	41.8	$2.3\cdot 10^{19}$	

Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on th English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

I have elected to leave BLEU out of the talk, but it's a measure of how good translation is and more is better

Also note the FLOPs difference relative to performance



LSTMs

Attention





### My unsolicited comments

**LSTMs** 

### Good stuff

- If you read machine learning literature, you know these models have revolutionized several fields
- There are some very cool tricks and innovations that I have struggled to highlight in this paper, notable how self attention masking can give you multiple independent gradients for in a single pass
- I like that "X is all you need" has become a meme title
- Transformer based models generate the best news headlines

#### ART IS IN THE AI OF THE BEHOLDER —

Machine Translation

### AI wins state fair art contest, annoys humans

Stealth win for AI-generated art inspires heated ethics debate on social media.

#### Not good stuff

- Training is great if you have a DGX A100 server lying around, but it took 2 days on my laptop to get through 20 epochs of 1000 before my laptop threw some OS error and killed it
- Self-attention across all inputs is an  $O(n^2)$  operation (all inputs attend to all other inputs), which can very extremely costly when you deal with things like images
- There is much in trying to solve the above problem such as the Performer, Linformer, and Reformer (great original names guys)
- Despite the technical innovations and contributions, the quality of Attention is all you need as a paper is f
   REDACTED

Attention



### Thanks for listening !

Feedback appreciated I am very inexperience at presenting technical content

see there's a typo!