Deep Learning Sequence to Sequence models: Attention Models

Sequence to sequence models





- Sequence goes in, sequence comes out
- No notion of "time synchrony" between input and output
 - May even not even maintain order of symbols
 - E.g. "I ate an apple" \rightarrow "Ich habe einen apfel gegessen"
 - Or even seem related to the input
 - E.g. "My screen is blank" \rightarrow "Please check if your computer is plugged in."

The "simple" translation model



- The recurrent structure that extracts the hidden representation from the input sequence is the *encoder*
- The recurrent structure that utilizes this representation to produce the output sequence is the *decoder*

A problem with this framework



- *All* the information about the input sequence is embedded into a *single* vector
 - The "hidden" node layer at the end of the input sequence
 - This one node is "overloaded" with information
 - Particularly if the input is long

A problem with this framework



- In reality: *All* hidden values carry information
 - Some of which may be diluted by the time we get to the final state of the encoder

A problem with this framework



- In reality: All hidden values carry information
 - Some of which may be diluted by the time we get to the final state of the encoder
- *Every* output is related to the input directly
 - Not sufficient to have the encoder hidden state to *only* the initial state of the decoder
 - Misses the direct relation of the outputs to the inputs



• Solution: Use a *different* weighted average for each output word

$$c_t = \frac{1}{N} \sum_{i}^{N} w_i(t) h_i$$



• Solution: Use a *different* weighted average for each output word

$$c_0 = \frac{1}{N} \sum_{i}^{N} w_i(0) h_i$$



• Solution: Use a *different* weighted average for each output word

$$c_1 = \frac{1}{N} \sum_{i}^{N} w_i(1)h_i$$



• Solution: Use a *different* weighted average for each output word

$$c_2 = \frac{1}{N} \sum_{i}^{N} w_i(2)h_i$$



• Solution: Use a *different* weighted average for each output word

$$c_3 = \frac{1}{N} \sum_{i}^{N} w_i(3)h_i$$



• Solution: Use a *different* weighted average for each output word

$$c_4 = \frac{1}{N} \sum_{i}^{N} w_i(4) h_i$$



• Solution: Use a *different* weighted average for each output word

$$c_5 = \frac{1}{N} \sum_{i}^{N} w_i(5)h_i$$



- This solution will work if the weights w_{ki} can somehow be made to "focus" on the right input word
 - E.g., when predicting the word "apfel", $w_3(4)$, the weight for "apple" must be high while the rest must be low
- How do we generate such weights??

Attention Models



- Attention weights: The weights w_i(t) are dynamically computed as functions of decoder state
 - Expectation: if the model is well-trained, this will automatically "highlight" the correct input
- But how are these computed?

Attention weights at time t



- The "attention" weights $w_i(t)$ at time t must be computed from available information at time t
- The primary information is s_{t-1} (the state at time time t-1)
 - Also, the input word at time t, but generally not used for simplicity

 $w_i(t) = a(\boldsymbol{h}_i, \boldsymbol{s}_{t-1})$

Requirement on attention weights



- The weights $w_i(t)$ must be positive and sum to 1.0
 - I.e. be a distribution
 - Ideally, they must be high for the most relevant inputs for the ith output and low elsewhere
- Solution: A two step weight computation
 - First compute raw weights (which could be +ve or -ve)
 - Then softmax them to convert them to a distribution

$$e_i(t) = g(\boldsymbol{h}_i, \boldsymbol{s}_{t-1})$$
$$w_i(t) = \frac{\exp(e_i(t))}{\sum_j \exp(e_j(t))}$$

Attention weights



Typical options for g() (variables in red must learned)

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = \mathbf{h}_{i}^{T} \mathbf{s}_{t-1}$$

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = \mathbf{h}_{i}^{T} \mathbf{W}_{g} \mathbf{s}_{t-1}$$

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = \mathbf{v}_{g}^{T} tanh\left(\mathbf{W}_{g} \begin{bmatrix} \mathbf{h}_{i} \\ \mathbf{s}_{t-1} \end{bmatrix}\right)$$

$$g(\mathbf{h}_{i}, \mathbf{s}_{t-1}) = MLP([\mathbf{h}_{i}, \mathbf{s}_{t-1}])$$

$$e_i(t) = g(\mathbf{h}_i, \mathbf{s}_{t-1})$$
$$w_i(t) = \frac{\exp(e_i(t))}{\sum_j \exp(e_j(t))}$$

Attention weights



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$$e_i(t) = g(\mathbf{h}_i, \mathbf{s}_{t-1})$$
$$w_i(t) = \frac{\exp(e_i(t))}{\sum_j \exp(e_j(t))}$$



• Pass the input through the encoder to produce hidden representations h_i



- Compute the attention weights $w_i(0)$ for the first output using s_{-1}
 - Will be a distribution over the input words
- Compute "context" c_0

 \leq SOS \geq

- Weighted sum of input word hidden states
- Input c₀ and <sos> to the decoder at time 0
 - <sos> because we are starting a new sequence
 - In practice we will enter the *embedding* of <sos>



The decoder computes

 y_0^{ich}

 $v_0^{\overline{du}}$

 y_0^{hat}

 \boldsymbol{Y}_0

- A probability distribution over the output vocabulary
 - Output of softmax output layer



 \boldsymbol{Y}_0 **s**₀ <sos> Sample a word from the output distribution

 y_0^{ich}

 y_0^{hat}

...

 y_0^{du}

Ich ___

 \boldsymbol{Y}_0

 $e_i(1) = g(\boldsymbol{h}_i, \boldsymbol{s}_0)$

 $w_i(1$

 $\frac{\exp(e_i(1))}{\sum_i \exp(e_i(1))} \quad c_1 = \frac{1}{N} \sum_{i=1}^{N} c_{i}$



- all inputs for the second output using s_0
 - Compute raw weights, followed by softmax
- Compute "context" c₁
 - Weighted sum of input hidden representations
- Input c₁ and first output word to the decoder
 - In practice we enter the *embedding* of the word

 $w_i(1)h_i$

Ν



- The decoder computes
 - *s*₁
 - A probability distribution over the output vocabulary

$$g(\mathbf{h}_i, \mathbf{s}_0) = \mathbf{h}_i^T \mathbf{W}_g \mathbf{s}_0$$

$$e_i(1) = g(\mathbf{h}_i, \mathbf{s}_0)$$

$$w_i(1) = \frac{\exp(e_i(1))}{\sum_j \exp(e_j(1))} \quad c_1 = \frac{1}{N} \sum_i^N w_i(1) h_i$$

$$q_3$$



 Sample the second word from the output distribution

$$g(\mathbf{h}_i, \mathbf{s}_0) = \mathbf{h}_i^T \mathbf{W}_g \mathbf{s}_0$$

$$e_i(1) = g(\mathbf{h}_i, \mathbf{s}_0)$$

$$w_i(1) = \frac{\exp(e_i(1))}{\sum_j \exp(e_j(1))} \quad c_1 = \frac{1}{N} \sum_i^N w_i(1) h_i$$

$$q_4$$







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$$e_{i}(4) = g(h_{i}, s_{3})$$

$$w_{i}(4) = \frac{\exp(e_{i}(4))}{\sum_{j} \exp(e_{j}(4))}$$

$$c_{4} = \frac{1}{N} \sum_{i}^{N} w_{i}(4)h_{i}$$



$$e_{i}(4) = g(h_{i}, s_{3})$$

$$w_{i}(4) = \frac{\exp(e_{i}(4))}{\sum_{j} \exp(e_{j}(4))}$$

$$c_{4} = \frac{1}{N} \sum_{i}^{N} w_{i}(4)h_{i}$$


Converting an input: Inference



$$e_{i}(5) = g(h_{i}, s_{4})$$

$$w_{i}(5) = \frac{\exp(e_{i}(5))}{\sum_{j} \exp(e_{j}(5))}$$

$$c_{5} = \frac{1}{N} \sum_{i}^{N} w_{i}(5)h_{i}$$

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Converting an input: Inference



Continue this process until <eos> is drawn

$$e_{i}(5) = g(h_{i}, s_{4})$$

$$w_{i}(5) = \frac{\exp(e_{i}(5))}{\sum_{j} \exp(e_{j}(5))} \qquad c_{5} = \frac{1}{N} \sum_{i}^{N} w_{i}(5)h_{i}$$

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Attention-based decoding



$$e_i(t) = g(\mathbf{h}_i, \mathbf{s}_{t-1})$$
$$w_i(t) = \frac{\exp(e_i(t))}{\sum_j \exp(e_j(t))}$$

$$c_t = \frac{1}{N} \sum_{i}^{N} w_i(t) h_i$$



- Encoder outputs an explicit "key" and "value" at each input time
 - Key is used to evaluate the importance of the input at that time, for a given output
- Decoder outputs an explicit "query" at each output time
 - Query is used to evaluate which inputs to pay attention to
- The weight is a function of key and query
- The actual context is a weighted sum of value

"Alignments" example: Bahdanau et al.



t

t

Plot of $w_i(t)$ Color shows value (white is larger)

Note how most important input words for any output word get automatically highlighted

The general trend is somewhat linear because word order is roughly similar in both languages

Extensions: Multihead attention



- Have multiple query/key/value sets.
 - Each attention "head" uses one of these sets
 - The combined contexts from all heads are passed to the decoder
- Each "attender" focuses on a different aspect of the input that's important for the decode

Some impressive results..

- Attention-based models are currently responsible for the state of the art in many sequence-conversion systems
 - Machine translation
 - Input: Text in source language
 - Output: Text in target language
 - Speech recognition
 - Input: Speech audio feature vector sequence
 - Output: Transcribed word or character sequence

Attention models in image captioning



A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.



A <u>stop</u> sign is on a road with a mountain in the background.



A little girl sitting on a bed with a teddy bear.

A group of <u>people</u> sitting on a boat in the water.

A giraffe standing in a forest with trees in the background.

- "Show attend and tell: Neural image caption generation with visual attention", Xu et al., 2016
- Encoder network is a convolutional neural network
 - Filter outputs at each location are the equivalent of h_i in the regular sequence-to-sequence model

Self attention



- First, for every word in the input sequence we compute an initial representation
 - E.g. using a single MLP layer

Self attention





- Then, from each of the hidden representations, we compute a query, a key, and a value.
 - Using separate linear transforms
 - The weight matrices W_q , W_k and W_v are learnable parameters



- For each word, we compute an attention weight between that word and all other words
 - The raw attention of the *i*th word to the *j*th word is a function of query q_i and key k_j
 - The raw attention values are put through a softmax to get the final attention weights



- The updated representation for the word is the attention-weighted sum of the values for all words
 - Including itself





- Compute query-key-value sets for every word
- For each word
 - Using the query for that word, compute attention weights for all words using their keys
 - Compute updated representation for the word as attention-weighted sum of values of all words



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- Compute query-key-value sets for every word
- For each word

 $q_i = \boldsymbol{W}_q h_i$

 $k_i = \boldsymbol{W}_k h_i$

 $v_i = W_v h_i$

- Using the query for that word, compute attention weights for all words using their keys
- Compute updated representation for the word as attention-weighted sum of values of all words



 $q_i = \boldsymbol{W}_q h_i$

 $k_i = \boldsymbol{W}_k h_i$

 $v_i = \boldsymbol{W}_v h_i$

This is a "single-head" self-attention block





- We can have *multiple* such attention "heads"
 - Each will have an independent set of queries, keys and values
 - Each will obtain an independent set of attention weights
 - Potentially focusing on a different aspect of the input than other heads
 - Each computes an independent output
- The final output is the concatenation of the outputs of these attention heads
- "MULTI-HEAD ATTENTION" (actually Multi-head self attention)

$$q_i^a = W_q^a h_i$$
$$\frac{k_i^a = W_k^a h_i}{v_i^a = W_v^a h_i}$$





• Multi-head self attention

- Multiple self-attention modules in parallel



- Typically, the output of the multi-head self attention is passed through one or more regular feedforward layers
 - Affine layer followed by a non-linear activation such as

ReLU Affine Layer is a fully connected layer (or dense layer) that performs a linear transformation followed by a bias addition.



MULTI-HEAD SELF ATTENTION BLOCK



 The entire unit, including multi-head selfattention module followed by MLP is a *multihead self-attention block*



MULTI-HEAD SELF ATTENTION BLOCK

 \boldsymbol{h}_2

an

 \boldsymbol{h}_3

apple

 h_4

<eos>



• The entire unit, including multi-head selfattention module followed by MLP is a *multi*head self-attention block



- The encoder can include many layers of such blocks
- No need for recurrence...



- Recap: The encoder in a sequence-to-sequence model can replace recurrence through a series of "multi-head self attention" blocks
- But this still ignores *relative position*
 - A context word one word away is different from one 10 words away
 - The attention framework does not take distance into consideration



• Note that the inputs are actually word *embeddings*



- Note that the inputs are actually word embeddings
- We add a "positional" encoding to them to capture the relative distance from one another

Positional Encoding

regenerate





- A vector of sines and cosines of a harmonic series of frequencies
 - Every 2*l*-th component of P_t is $\sin \omega_l t$
 - Every 2l + 1-th component of P_t is $\cos \omega_l t$
- Never repeats
- Has the linearity property required



• The linear relationship between P_t and $P_{t+\tau}$ enables the net to learn shift-invariant "gap" dependent relationships



• The self-attending encoder!!



• The self-attending encoder!!



 Self attention in encoder: Can use input embedding at time t+1 and further to compute output at time t, because all inputs are available

Self attention and masked self attention

- Self attention in decoder: Decoder is sequential
 - Each word is produced using the previous word as input
 - Only embeddings until time t are available to compute the output at time t
- The attention will have to be "masked", forcing attention weights for t+1 and later to 0





Transformer: Attention is all you need

Output

Vaswani, Ashish, et al. "Attention is all you need." *Advances in neural information processing systems*. 2017.



- Transformer: A sequence-to-sequence model that replaces recurrence with positional encoding and multi-head self attention
 - "Attention is all you need"
Transformer



From "Attention is all you need"

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

Model	BL	EU	Training C	Training Cost (FLOPs)			
Wodel	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	$9.6\cdot10^{18}$	$1.5\cdot 10^{20}$			
MoE [32]	26.03	40.56	$2.0\cdot 10^{19}$	$1.2\cdot 10^{20}$			
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Transformer (base model)	27.3	38.1	3.3 •	10 ¹⁸			
Transformer (big)	28.4	41.8	2.3	10^{19}			

- Transformer: tremendous decrease in model computation for similar performance as state-of-art translation models
- The last row in the table shows transformer performance
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Why so good?			W	/hy so fast

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Recap: Vanishing/exploding gradients



 $\nabla_{f_k} Div = \nabla D. \nabla f_N. W_N. \nabla f_{N-1}. W_{N-1} \dots \nabla f_{k+1} W_{k+1}$

- RNNs are just very deep networks
- LSTMs mitigate the problem at the cost of 3x more matrix multiplications
- Transformers get rid of it! To encode a full sentence, they have way fewer layers than an unrolled RNN.
- The same goes with the vanishing memory issue to an extent. 138



- Computing Y(T) requires Y(T-1)...
- Which requires Y(T-2), etc...
- RNN inputs must be processed in order \rightarrow slow implementation

Processing order



- q_n , k_n , v_n can be computed separately.
- $n^2 < q_n, k_n > \text{dot products to compute.}$
- Self attention is easy to compute in parallel → Faster implementations

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GPT



Alec Radford et. al., Improving Language Understanding by Generative Pre-Training

Table 5: Analysis of various model ablations on different tasks. Avg. score is a unweighted average of all the results. (mc= Mathews correlation, acc=Accuracy, pc=Pearson correlation)

Method	Avg. Score	CoLA (mc)	SST2 (acc)	MRPC (F1)	STSB (pc)	QQP (F1)	MNLI (acc)	QNLI (acc)	RTE (acc)
Transformer w/ aux LM (full)	74.7	45.4	91.3	82.3	82.0	70.3	81.8	88.1	56.0
Transformer w/o pre-training Transformer w/o aux LM LSTM w/ aux LM	59.9 75.0 69.1	18.9 47.9 30.3	84.0 92.0 90.5	79.4 84.9 83.2	30.9 83.2 71.8	65.5 69.8 68.1	75.7 81.1 73.7	71.2 86.9 81.1	53.8 54.4 54.6

- GPT uses only the decoder of the transformer as an LM — "Transformer w/o aux LM"
- Large performance improvement in many tasks

GPT



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- Add Task conditioning: put the nature of your task in the input (not just LM)
- Parameters x1000
- → GPT-3 : Generalizes to more tasks, not just more inputs!

BERT



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
BERT _{BASE}	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

Table 1: GLUE Test results, scored by the evaluation server (https://gluebenchmark.com/leaderboard). The number below each task denotes the number of training examples. The "Average" column is slightly different than the official GLUE score, since we exclude the problematic WNLI set.⁸ BERT and OpenAI GPT are single-model, single task. F1 scores are reported for QQP and MRPC, Spearman correlations are reported for STS-B, and accuracy scores are reported for the other tasks. We exclude entries that use BERT as one of their components.

- Bert: Only uses encoder of transformer to derive word and sentence embeddings
- Trained to "fill in the blanks"
- This is *representation learning* (more next lecture)

Attention is all you need

- Self-attention can effectively replace recurrence in sequence-to-sequence models
 - "Transformers"
 - Requires "positional encoding" to capture positional information
- Can also be used in regular sequence analysis settings as a substitute for recurrence
- Currently *the* state of the art in most sequence analysis/prediction...

Attention is all you need

- Self-attention can effectively replace recurrence in sequence-to-sequence models
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 - Requires "positional encoding" to capture positional information
- Can also be used in regular sequence analysis settings as a substitute for recurrence
- Currently *the* state of the art in most sequence analysis/prediction... and even computer vison problems!

Vision Transformers



Dosovitskiy et al, An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale, 2020

- Divide your image in patches with pos. encodings
- Apply Self-Attention!

→ Sequential and image problems are similar when using transformers

Impact of Transformers

- Transformers have played a major role in the "uniformization" of DL-based tasks:
 - Find a pretrained "BERT-like" transformer (Text, Image, Speech)
 - Fine-tune on your task or not! (Prompting...)
- This has helped democratize Deep Learning considerably



• But...

Caveat 1

- Not all transformers are the same: Big/small, fast/slow, mono-/multilingual, contrastive/ generative, regressive/autoencoding...
- Pick the right one!

Caveat 2

- Transformers are not always the right choice.
- They often require more parameters than LSTMs at equal performance
- → Tricky on small hardware (phones, IoT, etc)