BOSTON NIVERSITY

Deep Learning for Data Science DS 542

Lecture 15 Attention and Transformers

Slides originally by Thomas Gardos. Images from [Understanding Deep Learning](https://udlbook.com) unless otherwise cited.

A Brief History of Transformers

2000

Yoshua

Bengio*

A Neural Probabilistic

Language Model

 $C(w_{t-2})$ $C(w_t)$

Matrix C

across words

shared parameters

 $\bullet\bullet\bullet\bullet$

index for w_{t-2}

 $• •$

 $C(w_{t-n})$

Table

in C

 $look-up$

 $\bullet \bullet \bullet \bullet$

index for w_{t-n+1}

i-th output = $P(w_i = i | context)$

softmax

most computation here

tanh

 $\bullet\bullet\cdots\bullet$

index for w_{t-1}

 $\bullet\bullet\bullet$

*And others; Chronological analysis inspired by Andrej Karpathy's lecture, youtube.com/watch?v=XfpMkf4rD6E

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A Neural Probabilistic Language Model *Bengio et al, 2000 and 2003*

Figure 1: Neural architecture: $f(i, w_{t-1}, \dots, w_{t-n+1}) = g(i, C(w_{t-1}), \dots, C(w_{t-n+1}))$ where g is the neural network and $C(i)$ is the *i*-th word feature vector.

 $w_t \in V$ words in the vocabulary

- Build a probabilistic language model from NNs
- Feed forward network with shared parameters, C, that create embeddings
- Predicts the probability of a word at time t , based on the context of the last *n* words
- Can use shallow feed forward or recurrent neural networks

Limited to context length of n

Generating Sequences With Recurrent Neural Networks

By Graves, 2014

First use of neural networks for auto-regressive models?

- Predict next element of a sequence
- Such as next character, word, etc...

Familiar mapping from raw outputs to probabilities

$$
\Pr(x_{t+1} = k | y_t) = y_t^k = \frac{\exp(\hat{y}_t^k)}{\sum_{k'=1}^K \exp(\hat{y}_t^{k'})}
$$

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The ''Rebellion''' (''Hyerodent'') is [[literal]], related mildly older than old mad f sister, the music, and morrow been much more propellent. All those of [[H] ams (mass)|sausage trafficking]]s were also known as [[[Trip t of twelve years.)

By the 1978 Russian [[Turkey|Turkist]] conital city ceased by formers and the interior frame tend the interior tend to the tend of the station for Turkistion of movigation the ISBNs, all encoding [[Transylvania Internatio used.

Holding may be typically largely banned severish from sforked warhing tools and
behave laws, allowing the private jokes, even through missile IIC control, most
notably each, but no relatively larger success, is not being r rawn into forty-ordered cast and distribution.

Besides these markets (notably a son of humor).

Sometimes more or only lowed "80" to force a suit for http://news.bbc.
co.uk/1/sid9kcid/web/9960219.html ''[[#10:82-14]]''. <:blockguote>:

===The various disputes between Basic Mass and Council Conditioners - "Tita nist" class streams and anarchism===

Internet traditions sprang east with [[Southern neighborhood systems]] are improved with [[Nootbreaker]]s, bold hot missiles, its labor systems. [[KCD] numbere is stead former ISBN/MAS/speaker attacks "i:NS Skquoti, w

 $==$ See also $==$

Also Generated Handwriting Sequences

Training **Output**

(captured via smart whiteboard)

would find the bus safe and sound As for Hark, unless it was a canner at like ages of fifty-five Editorial. Dilemma of the the tides in the affairs of men;

Mar ay notion gow cargo there were egy med andre. Oxpertures that maine Cener le q hy maritre porner uiststaan sco linrel l'orpes 4 eald mainefs wine cases heint. I Coests the gagter me Neyle safet foning In soring Te a aver I hope earnice, Tend, hadp

Sequence to Sequence Learning with Neural **Networks**

Sutskever et al (2014)

Bottleneck

- Used LSTMs in an Encoder/Decoder structure
- Estimate the probability of $p(y_1, ..., y_{T'} | x_1, ..., x_T)$ where $T' \neq T$
- Encoder mapped sequence to a fixed size token (hidden state)
- The hidden state may not encode all the information needed by the decoder

Bottleneck between Encoder and Decoder!

I. Sutskever, O. Vinyals, and Q. V. Le, "Sequence to Sequence Learning with Neural Networks," in *Advances in Neural Information Processing Systems*, Curran Associates, Inc., 2014. [Link](https://proceedings.neurips.cc/paper/2014/hash/a14ac55a4f27472c5d894ec1c3c743d2-Abstract.html)

How to avoid that bottleneck? Attention!

Motivation:

- Arbitrarily far lookback
- Temporarily focus on certain inputs,
- And adjust focus based on output so far...

Attention Preview

L'accord sur la zone économique européenne a été signé en août 1992. <end>

The agreement on the European Economic Area was signed in August 1992. <end>

[https://jalammar.github.io/visualizing](https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/)[neural-machine-translation-mechanic](https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/) [s-of-seq2seq-models-with-attention/](https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/)

Neural Machine Translation by Jointly Learning to Align and **Translate** *Bahdanau, Cho & Bengio (2014-15)*

- Use bi-directional LSTMs to encode input
	- Read sequence forward and backward.
	- Save hidden states from each pass as "annotations" of the last read input.
- Attention model
	- Combine previous hidden state and each annotation separately.
	- Rescale attention via soft-max.
	- \circ Context vector = attention-weighted annotations

Neural Machine Translation by Jointly Learning to Align and Translate *Bahdanau, Cho & Bengio (2014-15)*

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	- Read sequence forward and backward.

Fixed

size

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Neural Machine Translation by Jointly Learning to Align and Translate *Bahdanau, Cho & Bengio (2014-15)*

- Automatically "soft-search" parts of input that influence the output
- Overcomes the bottleneck of a fixed size hidden state between encoder and decoder
- Significantly improved ability to comprehend longer sequences

Attention is All You Need *Vaswani et al (2017)*

- Removed LSTMs and didn't use convolutions
- Only attention mechanisms and MLP_S
- Parallelizable by removing sequential hidden state computation
- Outperformed all previous models

Transformers applied to many NLP applications

- Translation
- Question answering
- **•** Summarizing
- Generating new text
- Correcting spelling and grammar
- Finding entities
- Classifying bodies of text
- Changing style etc.

Transformers

- Motivation
- Dot-product self-attention
- Applying Self-Attention
- The Transformer Architecture
- Three Types of NLP Transformer Models

Design neural network to encode and process text:

The restaurant refused to serve me a ham sandwich, because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambience was just as good as the food and service.

Design neural network to encode and process text:

The restaurant refused to serve me a ham sandwich, because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambience was just as good as the food and service.

Encode word (or word parts) in some kind of D-dimensional embedding vector.

We'll look at tokenization and embedding encoding later.

For now assume a word is a token.

Design neural network to encode and process text:

The restaurant refused to serve me a ham sandwich, because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambience was just as good as the food and service.

Normally we would represent punctuation, capitalization, spaces, etc. as well.

Standard fully-connected layer

Standard fully-connected layer

$$
\mathbf{h} = \mathbf{a}[\boldsymbol{\beta} + \boldsymbol{\Omega} \mathbf{x}]
$$

Problem:

- token (word) vectors may be 512 or 1024 dimensional
- need to process large segment of text
- Hence, would require a very large number of parameters
- Can't cope with text of different lengths

Conclusion:

• We need a model where parameters don't increase with input length

Design neural network to encode and process text:

The (restaurant) refused to serve me a ham sandwich, because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambience was just as good as the food and service.

The word their must "attend to" the word restaurant.

Design neural network to encode and process text:

The (restaurant) refused to serve me a ham sandwich, because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambience was just as good as the food and service.

The word their must "attend to" the word restaurant.

Conclusions:

- There must be connections between the words.
- The strength of these connections will depend on the words themselves.

- Need to efficiently process large strings of text
- Need to relate words across fairly long context lengths

Self-Attention addresses these problems

Transformers

- Motivation
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- 1. Shares parameters to cope with long input passages of different lengths
- 2. Contains connections between word representations that depend on the words themselves

- Takes N inputs of size Dx1 and returns N inputs of size Dx1
- Computes N values (no ReLU)

$$
\mathbf{v}_n = {\boldsymbol{\beta}}_v + \mathbf{\Omega}_v \mathbf{x}_n
$$

• N outputs are weighted sums of these values

- Takes N inputs of size Dx1 and returns N inputs of size Dx1
- Computes N values (no ReLU)

$$
\mathbf{v}_n = {\boldsymbol{\beta}}_v + \mathbf{\Omega}_v \mathbf{x}_n
$$

• N outputs are weighted sums of these values

$$
\mathbf{sa}[\mathbf{x}_n] = \sum_{m=1}^N a[\mathbf{x}_n, \mathbf{x}_m] \mathbf{v}_m
$$
Dot product name from this expression

- Takes N inputs of size Dx1 and returns N inputs of size Dx1
- Computes N values (no ReLU)

$$
\mathbf{v}_n = \boldsymbol{\beta}_v + \boldsymbol{\Omega}_v \mathbf{x}_n
$$

Scalar self-attention weights that N outputs are weighted sums of these values represent how much attention the *n th* token should pay to the *mth* token $\mathbf{sa}_n[\mathbf{x}_1,\ldots,\mathbf{x}_N] = \sum_{n=1}^{N} a[\mathbf{x}_m,\mathbf{x}_n] \mathbf{v}_m.$ $m=1$ $a[\cdot, \mathbf{x}_n]$ are non-negative and sum to one

Here:

of inputs, $N = 3$

Dimension of each input, $D = 4$

We'll show how to calculate the self-attention weights shortly.

Attention weights

• Compute N "queries" and N "keys" from input

$$
\mathbf{q}_n = \boldsymbol{\beta}_q + \boldsymbol{\Omega}_q \mathbf{x}_n
$$

$$
\mathbf{k}_n = \boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{x}_n,
$$

• Calculate similarity and pass through softmax:

$$
a[\mathbf{x}_n, \mathbf{x}_m] = \text{softmax}_m [\text{sim}[\mathbf{k}_m \mathbf{q}_n]]
$$

$$
= \frac{\exp [\text{sim}[\mathbf{k}_m \mathbf{q}_n]]}{\sum_{m'=1}^{N} \exp [\text{sim}[\mathbf{k}'_m \mathbf{q}_n]]}
$$

● Weights depend on the inputs themselves

Attention weights

• Compute N "queries" and N "keys" from input

$$
\mathbf{q}_n = \boldsymbol{\beta}_q + \boldsymbol{\Omega}_q \mathbf{x}_n
$$

$$
\mathbf{k}_n = \boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{x}_n,
$$

• Take dot products and pass through softmax:

$$
a[\mathbf{x}_n, \mathbf{x}_m] = \text{softmax}_m [\mathbf{k}_m^T \mathbf{q}_n]
$$

$$
= \frac{\exp [\mathbf{k}_m^T \mathbf{q}_n]}{\sum_{m'=1}^N \exp [\mathbf{k}_{m'}^T \mathbf{q}_n]}
$$

Dot product = measure of similarity

A drawback of the dot product as similarity measure is the magnitude of each vector influences the value. More rigorous to divide by magnitudes.

Cosine Similarity:
$$
\frac{x^T y}{|x||y|} = \cos(\theta)
$$

Design neural network to encode and process text:

The restaurant refused to serve me a ham sandwich, because it only cooks vegetarian food. In the end, they just gave me two slices of bread. Their ambience was just as good as the food and service.

Conclusions:

We need a model where parameters don't increase with input length, e.g.

$$
\boldsymbol{\phi} = \{\boldsymbol{\beta}_v, \boldsymbol{\Omega}_v, \boldsymbol{\beta}_q, \boldsymbol{\Omega}_q, \boldsymbol{\beta}_k, \boldsymbol{\Omega}_k\}
$$

There must be connections between the words.

The strength of these connections will depend on the words themselves.

Ok, we defined *queries*, *keys* and *values*, but how are they used?
- Motivation
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Computing Attention Weights

$$
a[\mathbf{x}_n, \mathbf{x}_m] = \text{softmax}_m \left[\mathbf{k}_m^T \mathbf{q}_n \right]
$$

Computing Values and Self-Attention Outputs as Sparse Matrix **Ops**

From Input Vector to Input Matrix

• Store N input vectors in matrix X

• Compute values, queries and keys:

$$
\mathbf{V}[\mathbf{X}] = \boldsymbol{\beta}_v \mathbf{1}^{\mathbf{T}} + \mathbf{\Omega}_{\mathbf{v}} \mathbf{X}
$$

$$
\mathbf{Q}[\mathbf{X}] = \boldsymbol{\beta}_q \mathbf{1}^{\mathbf{T}} + \mathbf{\Omega}_{\mathbf{q}} \mathbf{X}
$$

$$
\mathbf{K}[\mathbf{X}] = \boldsymbol{\beta}_k \mathbf{1}^{\mathbf{T}} + \mathbf{\Omega}_{\mathbf{k}} \mathbf{X},
$$

• Combine self-attentions

$$
\mathbf{Sa}[\mathbf{X}] = \mathbf{V}[\mathbf{X}] \cdot \mathbf{Softmax}\Big[\mathbf{K}[\mathbf{X}]^T \mathbf{Q}[\mathbf{X}]\Big] = \mathbf{V} \cdot \mathbf{Softmax}\big[\mathbf{K}^T \mathbf{Q}\big]
$$

Scaled Dot Product Self-Attention

To avoid the case where a large value dominates the softmax in

$$
\mathbf{Sa}[\mathbf{X}] = \mathbf{V}\cdot\mathbf{Softmax}[\mathbf{K}^T\mathbf{Q}]
$$

you can scale the dot product by the square root of the dimension of the query $\textbf{Sa}[\textbf{X}] = \textbf{V} \cdot \textbf{Softmax}\left[\frac{\textbf{K}^T\textbf{Q}}{\sqrt{D}_q} \right]$

Put it all together in matrix form

Put it all together in matrix form

Put it all together in matrix form

attention weights scales quadratically with sequence length, N, but independent of length D of each input

Linear combination of weighted inputs where weights calculated from nonlinear functions

Hypernetwork – 1 branch calculates weights of other branch

Multi-Head Self Attention

- Multiple self-attention heads are usually applied in parallel
- "allows model to jointly attend to info from different representation subspaces at different positions"
- Original paper used 8 heads
- All can be executed in parallel

A function f[x] is equivariant to a transformation t[] if: $f[t[x]] = t[f[x]]$

Equivariance to Word Order

Self-attention is *equivariant* to permuting word order. Just a bag of words.

But word order is important in language:

The man ate the fish vs. The fish ate the man

Solution: Position Encoding

Idea is to somehow encode *absolute* or *relative* position in the inputs

> Fourier features used in neural fields are a version of this idea.

Absolute Position encoding

 \mathbf{H}

Add some matrix, Π , to the $D \times N$ input matrix:

T can be pre-defined or learned

Absolute Position encoding

Alternatively, could be added to each layer

 $S\mathbf{a}[\mathbf{X}] = \mathbf{V} \cdot \mathbf{Softmax}[\mathbf{K}^T \mathbf{Q}]$

$\textbf{Sa}[\textbf{X}] = (\textbf{V} + \boldsymbol{\Pi}) \cdot \textbf{Softmax}[(\textbf{K} + \boldsymbol{\Pi})^T (\textbf{Q} + \boldsymbol{\Pi})^T]$

Relative Position Encoding

Absolute position of a word is less important than relative position between inputs

Each element of the attention matrix corresponds to an offset between query position a and key position b

Learn a parameter $\pi_{a,b}$ for each offset and modify Attention[a,b] in some way.

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- The Transformer Architecture
- Three Types of NLP Transformer Models

● Multi-headed Self Attention is just one component of the transformer architecture

- *● Multi-headed Self Attention* is just one component of the transformer architecture
- ●Let's look at a transformer *block* (or *layer*) from the encoder

Transformer Layer -- Complete

- Adds a 2-layer MLP
- Adds residual connections around multi-head self-attentions and the parallels MLPs
- Adds LayerNorm, which normalizes across all the N input samples

Transformer Layer -- MLP

-
- Adds 2-layer MLP Same network (same weights) operates independently on each word
	- Learn more complex representations and expand model capacity

Linear_{Dx4D} \Box ReLU(.) \Box Linear_{4DxD}

Transformer Layer -- LayerNorm

- Normalize across same layer
- Learned gain and offset

NLP Example

57 batch, sentence_length, embedding_dim = 20, 5, 10 embedding = torch.randn(batch, sentence_length, embedding_dim) layer_norm = nn.LayerNorm(embedding_dim)

Activate module layer_norm(embedding)

Calculated column-wise <https://pytorch.org/docs/stable/generated/torch.nn.LayerNorm.html>

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3 Types of Transformer Models

- *1. Encoder* transforms text embeddings into representations that support variety of tasks (e.g. sentiment analysis, classification)
	- ❖ Model Example: BERT
- *2. Decoder* predicts the next token to continue the input text (e.g. ChatGPT, AI assistants)
	- ❖ Model Example: GPT4, GPT4
- *3. Encoder-Decoder* used in sequence-to-sequence tasks, where one text string is converted to another (e.g. machine translation)

Encoder Model Example: BERT (2019) *Bidirectional Encoder Representations from Transformers*

Hyperparameters

- 30,000 token vocabulary
- 1024-dimensional word embeddings
- 24x transformer layers
- 16 heads in self-attention mechanism
- \circ 4096 hidden units in middle of MLP
- \sim 340 million parameters
- Pre-trained in a self-supervised manner,
- then can be adapted to task with one additional layer and fine-tuned

This is a popular model to fine-tune for specialized tasks.

J. Devlin, M.-W. Chang, K. Lee, and K. Toutanova, "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding." arXiv, May 24, 2019. doi: [10.48550/arXiv.1810.04805.](https://doi.org/10.48550/arXiv.1810.04805)

Encoder Pre-Training

- A small percentage of input embedding replaced with a generic <mask> token
- Predict missing token from output embeddings
- Added linear layer and softmax to generate probabilities over vocabulary
- Trained on BooksCorpus (800M words) and English Wikipedia (2.5B) words)

- Extra layer(s) appended to convert output vectors to desired output format
- 3rd Example: Text span prediction -- predict start and end location of answer to a question in passage of Wikipedia, see<https://rajpurkar.github.io/SQuAD-explorer/>

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Decoder Model Example: GPT3 (2020) *Generative Pre-trained Transformer*

- One purpose: generate the next token in a sequence
- By constructing an autoregressive model

We saw this interface before, but better internals now.

Decoder Model Example: GPT3 (2020) *Generative Pre-trained Transformer*

- One purpose: generate the next token in a sequence
- By constructing an autoregressive model
- Factors the probability of the sentence: $Pr(Learning deep learning is fun) =$ $Pr(Learning) \times Pr(deep | learning) \times$ $Pr(learning \mid Learning \text{ deep}) \times$ $Pr(is \mid Learning\text{ deep learning}) \times$ $Pr(fun|Learning deep learning is)$

Decoder Model Example: GPT3 (2020) *Generative Pre-trained Transformer*

- One purpose: generate the next token in a sequence
- By constructing an autoregressive model
- Factors the probability of the sentence: $Pr(Learning deep learning is fun) =$ $Pr(Learning) \times Pr(deep| learning) \times$ $Pr(learning| Learning deep) \times$ $Pr(is | Learning deep learning) \times$ $Pr(fun|Learning\text{ deep learning is})$
- More formally: Autoregressive model $_N$

$$
Pr(t_1, t_2, ..., t_N) = Pr(t_1) \prod_{n=2} Pr(t_n | t_1, t_2, ..., t_{n-1})
$$

T. B. Brown *et al.*, "Language Models are Few-Shot Learners." arXiv, Jul. 22, 2020. doi: [10.48550/arXiv.2005.14165](https://doi.org/10.48550/arXiv.2005.14165).

Decoder: *Masked* Self-Attention

- During training we want to maximize the log probability of the input text under the autoregressive model
- We want to make sure the model doesn't "cheat" during training by looking ahead at the next token
- Hence we mask the self attention weights corresponding to current and right context to negative infinity

Masked Self-Attention

Mask right context self-attention weights to zero

Decoder: Text Generation (Generative AI)

- Prompt with token string "<start> It takes great"
- Generate next token for the sequence by
	- picking most likely token
	- sample from the probability distribution
		- alternative top-k sampling to avoid picking from the long tail
	- beam search select the most likely sentence rather than greedily pick
Decoder: Text Generation (Generative AI)

• Feed the output back into input

Decoder: Text Generation (Generative AI)

• Feed the output back into input

Technical Details

Again, BERT is viable and available for your projects.

Transformers

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Encoder-Decoder Model

• Used for machine translation, which is a sequence-to-sequence task

Decoder only continues input sequences.

Encoder-decoder produces new sequences based on input sequences.

<https://jalammar.github.io/illustrated-transformer/>

Encoder Decoder Model

- The transformer layer in the decoder of the encoder-decoder model has an extra stage
- Attends to the input of the encoder with cross attention using Keys and Values from the output of the encoder
- Shown here on original diagram from "Attention is all you need" paper

Encoder Decoder Model

• Same view per UDL book

Cross-Attention

Feedback?

