# CS 307 Modeling and Learning in Data Science

# Today's goal

- Recall:
  - Image autoencoder
  - Simple word embeddings
  - Encoder decoder for word embeddings
  - Attention
  - Transformers
- BERT
- GPT

# Sequence-to-sequence is everywhere!

- Sequence-to-sequence is useful for *more than just MT*
- Many NLP tasks can be phrased as sequence-to-sequence:
  - Summarization (long text  $\rightarrow$  short text)
  - Dialogue (previous utterances  $\rightarrow$  next utterance)
  - Parsing (input text  $\rightarrow$  output parse as sequence)
  - Code generation (natural language  $\rightarrow$  Python code)

• Vinyals et al., 2015











Converting tree to sequence



 $(S (NP NNP)_{NP} (VP VBZ (NP DT NN)_{NP})_{VP}.)_{S}$ 

Converting tree to sequence



 $(NP NNP)_{NP} (VP VBZ (NP DT NN)_{NP})_{VP}.)_{S}$ 

#### Model



#### Results



# Attention is a *general* Deep Learning technique

- More general definition of attention
  - Given a set of vector values, and a vector query, attention is a technique to compute a weighted sum of the values, dependent on the query.
  - We sometimes say that the query *attends to* the values
  - For example, in the seq2seq + attention model, each decoder hidden state attends to the encoder hidden states



#### Attention is all you need? – Transformer Networks

**English German Translation quality** 



Problems with RNNs = Motivation for Transformers

- Recurrent models typically factor computation along the symbol positions of the input and output sequences
  - Sequential computation prevents parallelization
  - Critical at longer sequence lengths, as memory constraints limit batching across examples
- Despite advanced RNNs like LSTMs, RNNs still need attention mechanism to deal with long range dependencies – path length for codependent computation between states grows with sequence
- But if attention gives us access to any state... maybe we don't need the RNN?

# Transformer Overview Recall

- Sequence-to-sequence
- Encoder-Decoder
- Task: machine translation with parallel corpus
- Predict each translated word
- Final cost/error function is standard cross-entropy error on top of a softmax classifier



# Transformer Basics

• Let's define the basic building blocks of transformer networks first: new attention layers!

Dot-Product Attention (Extending our previous def.)

- Inputs: a query q and a set of key-value (k-v) pairs to an output
  - Query, keys, values, and output are all vectors
- Output is weighted sum of values, where
  - Weight of each value is computed by an inner product of query and corresponding key
  - Queries and keys have same dimensionality

$$A(q, K, V) = \sum_{i} \frac{e^{q \cdot k_i}}{\sum_{j} e^{q \cdot k_j}} v_i$$

#### Dot-Product Attention – Matrix notation

• When we have multiple queries q, we stack them in a matrix Q:

$$A(q, K, V) = \sum_{i} \frac{e^{q \cdot k_i}}{\sum_{j} e^{q \cdot k_j}} v_i$$

• Becomes:

$$A(Q,K,V) = softmax(QK^T)V$$



- Problem: As d<sub>k</sub> gets large, the variance of q<sup>T</sup>k increases → some values inside the softmax get large → the softmax gets very peaked → hence its gradient gets smaller.
- Solution: Scale by length of query/key vectors:

$$A(Q, K, V) = softmax \left(\frac{QK^T}{\sqrt{d_k}}\right) V$$



# Self-attention and Multi-head attention

- The input word vectors could be the queries, keys and values
  - In other words: the word vectors themselves select each other
  - Word vector stack = Q = K = V
- Problem: Only one way for words to interact with one-another
- Solution: Multi-head attention
  - First map Q, K, V into h many lower dimensional spaces via W matrices
  - Then apply attention, then concatenate outputs and pipe through linear layer

MultiHead
$$(Q, K, V)$$
 = Concat(head<sub>1</sub>, ..., head<sub>h</sub>) $W^{O}$   
where head<sub>i</sub> = Attention $(QW_{i}^{Q}, KW_{i}^{K}, VW_{i}^{V})$ 



## Self-Attention



(example and picture from David Talbot)

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





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





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

























# Complete transformer block

- Each block has two "sublayers"
  - 1. Multihead attention
  - 2. 2 layer feed-forward Nnet (with relu)



- Residual (short-circuit) connection and LayerNorm:
- LayerNorm(x + Sublayer(x))<sup>2</sup>
  - Layernorm changes input to have mean 0 and variance 1, per layer and per training point (and adds two more parameters)

$$\mu^{l} = rac{1}{H} \sum_{i=1}^{H} a_{i}^{l} \qquad \sigma^{l} = \sqrt{rac{1}{H} \sum_{i=1}^{H} \left(a_{i}^{l} - \mu^{l}
ight)^{2}} \qquad \qquad h_{i} = f(rac{g_{i}}{\sigma_{i}} \left(a_{i} - \mu_{i}
ight) + b_{i})$$

Add & Norm

Feed

Forward

Add & Norm

Multi-Head Attention



# Encoder Input

- Actual word representations are byte-pair encodings
  - Rico Sennrich, Barry Haddow, and Alexandra Birch. Neural Machine Translation of Rare Words with Subword Units. ACL 2016.
- Added is a positional encoding so same words at different locations have different overall representations:

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

*pos* is the position of a word *i* is the dimension index


# Self Attention Visualization in Layer 5

• Words start to pay attention to other words in sensible ways



# Transformer Decoder

- 2 sublayer changes in decoder
- Masked decoder self-attention
  - Only depends on previous words
- Encoder-Decoder Attention
  - Queries come from previous decoder layer and keys and values come from output of encoder





# Advantages

- No recurrence: parallel encoding
- Fast training: both encoder and decoder are parallel
- No long range problem: O(1) for all tokens direct connections
- Three attentions: the model does not have to remember too much
- Multi-head attention allows to pay attention to different aspects
- Why self-attention and CNN is better than RNN on NMT is still under investigation



# Avoid Information Bottleneck



# Last time we introduced transformer



## Transformers, GPT-2, and BERT

- 1. A transformer uses Encoder stack to model input, and uses Decoder stack to model output (using input information from encoder side).
- 2. But if we do not have input, we just want to model the "next word", we can get rid of the Encoder side of a transformer and output "next word" one by one. This gives us GPT.
- 3. If we are only interested in training a language model for the input for some other tasks, then we do not need the Decoder of the transformer, that gives us BERT.





Model Dimensionality: 768

Model Dimensionality: 1024

Model Dimensionality: 1280

Model Dimensionality: 1600

#### GPT-2 in action



## Byte Pair Encoding (BPE)

Word embedding sometimes is too high level, pure character embedding too
low level. For example, if we have learned
old older oldest
We might also wish the computer to infer
smart smarter smartest

But at the whole word level, this might not be so direct. Thus the idea is to break the words up into pieces like er, est, and embed frequent fragments of words.

GPT adapts this BPE scheme.

### Byte Pair Encoding (BPE)

GPT uses BPE scheme. The subwords are calculated by:

- 1. Split word to sequence of characters (add </w> char)
- 2. Joining the highest frequency pattern.
- 3. Keep doing step 2, until it hits the pre-defined maximum number of sub-words or iterations.

Example (5, 2, 6, 3 are number of occurrences) {'l o w </w>': 5, 'l o w e r </w>': 2, 'n e w e s t </w>': 6, 'w i d e s t </w>': 3 } {'l o w </w>': 5, 'l o w e r </w>': 2, 'n e w est </w>': 6, 'w i d est </w>': 3 } {'l o w </w>': 5, 'l o w e r </w>': 2, 'n e w est </w>': 6, 'w i d est </w>': 3 } (est freq. 9) {'lo w </w>': 5, 'lo w e r </w>': 2, 'n e w est</w>': 6, 'w i d est</w>': 3 } (lo freq 7) Masked Self-Attention (to compute more efficiently)



#### Masked Self-Attention



## Masked Self-Attention Calculation

Re-use previous computation results: at any step, only need to results of q, k, v related to the new output word, no need to re-compute the others. Additional computation is linear, instead of quadratic.

#### GPT-2 fully connected network has two layers (Example for GPT-2 small)



GPT-2 has a parameter top-k, so that we sample words from top

k (highest probability from softmax) words for each output





#### This top-k parameter, if k=1, we would have output like:

The first time I saw the new version of the game, I was so excited. I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of the game, I was so excited to see the new version of

# **GPT** Training

GPT-2 uses unsupervised learning approach to training the language model.

There is no custom training for GPT-2, no separation of pre-training and fine-tuning like BERT.

#### A story generated by GPT-2

"The scientist named the population, after their distinctive horn, Ovid's Unicorn. These fourhorned, silver-white unicorns were previously unknown to science.

Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.

Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.

Pérez and the others then ventured further into the valley. 'By the time we reached the top of one peak, the water looked blue, with some crystals on top,' said Pérez.

Pérez and his friends were astonished to see the unicorn herd. These creatures could be seen from the air without having to move too much to see them – they were so close they could touch their horns."

# Transformer / GPT prediction



### **GPT-2** Application: Translation

#### **Training Dataset**

| I    | am      | а               | student | <to-fr></to-fr> | je     | suis    | étudiant |
|------|---------|-----------------|---------|-----------------|--------|---------|----------|
| let  | them    | eat             | cake    | <to-fr></to-fr> | Qu'ils | mangent | de       |
| good | morning | <to-fr></to-fr> | Bonjour |                 |        |         |          |



#### **GPT-2** Application: Summarization



## Using wikipedia data

| 3   |  |  |   |  |  |   | -   | -   | Report William  |   |
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| Aş  | positronic brain is a fiction  | onal technologic   | al device, original   | ly conceived by so   | cience fiction writer  | Isaac As  | imov. <sup>j</sup> 1  | [2] It functions  | as a central proce  | essing unit (CPU) for   |
| rob   | bots, and, in some unspec  | ified way, provi   | des them with a fo  | orm of consciousne   | ess recognizable to  | humans  | When  | Asimov wrote  | his first robot stor  | les in 1939 and 194   |
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|   | 3.3 Doctor Who   |  |   |  |  |   |   |   |   |   |
| a   | 3.4 Star Trek  |  |   |  |  |   |   |   |   |   |
|   | 3.5 Peny Rhodan  |  |   |  |  |   |   |   |   |   |
|   | 3.6 CHOBOC 2004 Pain<br>3.7 Dicentennial Man   |  |   |  |  |   |   |   |   |   |
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# How about representation/word embedding?

#### BERT (Bidirectional Encoder Representation from Transformers)



Model input dimension 512

#### Input and output vector size



BERT

# Pre-training in NLP

- Word embeddings are the basis of deep learning for NLP
- Word embeddings (word2vec, GloVe) are often *pre-trained* on text corpus from co-occurrence statistics
- **Problem**: Word embeddings are applied in a context free manner



• Solution: Train contextual representations on text corpus

# History of Contextual Representations

• Semi-Supervised Sequence Learning, Google, 2015



# History of Contextual Representations

• *ELMo: Deep Contextual Word Embeddings*, AI2 & University of Washington, 2017



• Improving Language Understanding by Generative Pre-Training, OpenAl, 2018 (GPT)



# Problem with Previous Methods

- **Problem**: Language models only use left context *or* right context, but language understanding is bidirectional.
- Why are LMs unidirectional?
  - Reason 1: Directionality is needed to generate a well-formed probability distribution.
    - We don't care about this.
  - Reason 2: Words can "see themselves" in a bidirectional encoder.

# Unidirectional vs. Bidirectional Models

Unidirectional context Build representation incrementally



**Bidirectional context** Words can "see themselves"



# Masked LM

- Solution: Mask out k% of the input words, and then predict the masked words
  - We always use *k* = 15%



- Too little masking: Too expensive to train
- Too much masking: Not enough context

# Masked LM

- Problem: Mask token never seen at fine-tuning
- Solution: 15% of the words to predict, but don't replace with [MASK] 100% of the time. Instead:
  - 80% of the time, replace with [MASK]
    - went to the store  $\rightarrow$  went to the [MASK]
  - 10% of the time, replace random word
    - went to the store  $\rightarrow$  went to the running
  - 10% of the time, keep same
    - went to the store  $\rightarrow$  went to the store

# Next Sentence Prediction

• To learn *relationships* between sentences, predict whether Sentence B is actual sentence that proceeds Sentence A, or a random sentence

Sentence A = The man went to the store.
Sentence B = He bought a gallon of milk.
Label = IsNextSentence

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

# **BERT** pretraining

ULM-FiT (2018): Pre-training ideas, transfer learning in NLP. ELMo: Bidirectional training (LSTM)

Transformer: Although used things from left, but still missing from the right.

GPT: Use Transformer Decoder half.

**BERT:** Switches from Decoder to Encoder, so that it can use both sides in training and invented corresponding training tasks: masked language model
# BERT Pretraining Task 1: masked words



## BERT Pretraining Task 2: two sentences



## BERT Pretraining Task 2: two sentences



50% true second sentences 50% random second sentences

# Fine-tuning BERT for other specific tasks

#### MNLI

- QQP (Quaro Question Pairs) Semantic equivalence) QNLI (NL inference dataset) STS-B (texture similarity) MRPC (paraphrase, Microsoft) RTE (textual entailment) SWAG (commonsense inference) SST-2 (sentiment)
- CoLA (linguistic acceptability SQuAD (question and answer)

- Class Label C T, ... T<sub>N</sub> T<sub>[SEP]</sub> T, ... T<sub>M</sub> BERT E<sub>[0.5]</sub> E<sub>1</sub> ... E<sub>N</sub> E<sub>[SEP]</sub> E<sub>1</sub> ... E<sub>M</sub> C T, ... T<sub>M</sub> BERT E<sub>[0.5]</sub> E<sub>1</sub> ... E<sub>N</sub> E<sub>[SEP]</sub> E<sub>1</sub> ... E<sub>M</sub> C T<sub>1</sub> ... T<sub>M</sub> Sentence 1 Sentence 2
- (a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG



(c) Question Answering Tasks: SQuAD v1.1



(b) Single Sentence Classification Tasks: SST-2, CoLA



(d) Single Sentence Tagging Tasks: CoNLL-2003 NER SST (Stanford sentiment treebank): 215k phrases with fine-grained sentiment labels in the parse trees of 11k sentences.

## NLP Tasks: Multi-Genre Natural Lang. Inference

| -  |  |   |  |
|--|--|---|--|
| MNLI: 433k<br>pairs of<br>examples,                    | Met my first girlfriend that way.  | Face-to-Face<br><b>contradiction</b><br>C C N C | I didn't meet my first girlfriend until later.   |
|  | 8 million in relief in the form of emergency housing.  | GOVERNMENT<br>neutral<br>N N N N                | The 8 million dollars for emergency hous-<br>ing was still not enough to solve the prob-<br>lem. |
| labeled by<br>entailment,<br>neutral or<br>contraction | Now, as children tend their gardens, they have a new ap-<br>preciation of their relationship to the land, their cultural<br>heritage, and their community. | Letters<br><b>neutral</b><br>N N N N            | All of the children love working in their gardens.   |
|  | At 8:34, the Boston Center controller received a third transmission from American 11   | 9/11<br>entailment<br>E E E E                   | The Boston Center controller got a third transmission from American 11.                          |
|  | I am a lacto-vegetarian.   | SLATE<br>neutral<br>N N E N                     | I enjoy eating cheese too much to abstain from dairy.  |
|  | someone else noticed it and i said well i guess that's true<br>and it was somewhat melodious in other words it wasn't<br>just you know it was really funny | Telephone<br>contradiction<br>C C C C           | No one noticed and it wasn't funny at all.   |

Table 1: Randomly chosen examples from the development set of our new corpus, shown with their genre labels, their selected gold labels, and the validation labels (abbreviated E, N, C) assigned by individual annotators.

### **NLP Tasks** (SQuAD -- Stanford Question Answering Dataset):

Sample: Super Bowl 50 was an American football game to determine the champion of the National Football League (NFL) for the 2015 season. The American Football Conference (AFC) champion Denver Broncos defeated the National Football Conference (NFC) champion Carolina Panthers 24–10 to earn their third Super Bowl title. The game was played on February 7, 2016, at Levi's Stadium in the San Francisco Bay Area at Santa Clara, California. As this was the 50th Super Bowl, the league emphasized the "golden anniversary" with various gold-themed initiatives, as well as temporarily suspending the tradition of naming each Super Bowl game with Roman numerals (under which the game would have been known as "Super Bowl L"), so that the logo could prominently feature the Arabic numerals 50.

Which NFL team represented the AFC at Super Bowl 50?

Ground Truth Answers: Denver Broncos

Which NFL team represented the NFC at Super Bowl 50?

Ground Truth Answers: Carolina Panthers

#### SegaTron/SegaBERT



Figure 1: Input Representation of SegaBERT

H. Bai, S. Peng, J. Lin, L. Tan, K. Xiong, W. Gao, M. Li: SgaTron: Segment-aware transformer for language modeling and understanding. AAAI'2021



Figure 2: Valid perplexities and losses during the training processes of language modeling and pre-training.

|                        | BASE model(wikipedia 500K steps) |          |      | LARGE model(wikibooks 1000K steps) |      |          |      |          |
|------------------------|----------------------------------|----------|------|------------------------------------|------|----------|------|----------|
| Task(Metrics)          | dev                              |          | test |                                    | dev  |          | test |          |
|                        | BERT                             | SegaBERT | BERT | SegaBERT                           | BERT | SegaBERT | BERT | SegaBERT |
| CoLA (Matthew Corr.)   | 55.0                             | 54.7     | 43.5 | 50.7                               | 60.6 | 65.3     | 60.5 | 62.6     |
| SST-2 (Acc.)           | 91.3                             | 92.1     | 91.2 | 91.5                               | 93.2 | 94.7     | 94.9 | 94.8     |
| MRPC (F1)              | 92.6                             | 92.4     | 88.9 | 89.3                               | -    | 92.3     | 89.3 | 89.7     |
| STS-B (Spearman Corr.) | 88.9                             | 89.0     | 83.9 | 84.6                               | _    | 90.3     | 86.5 | 88.6     |
| QQP (F1)               | 86.5                             | 87.0     | 70.8 | 71.4                               | -    | 89.1     | 72.1 | 72.5     |
| MNLI-m (Acc.)          | 83.2                             | 83.8     | 82.9 | 83.5                               | 86.6 | 87.6     | 86.7 | 87.9     |
| MNLI-mm (Acc.)         | 83.4                             | 84.1     | 82.8 | 83.2                               | -    | 87.5     | 85.9 | 87.7     |
| QNLI (Acc.)            | 90.4                             | 91.5     | 90.1 | 90.8                               | 92.3 | 93.6     | 92.7 | 94.0     |
| RTE (Acc.)             | 68.3                             | 71.8     | 65.4 | 68.1                               | 70.4 | 78.3     | 70.1 | 71.6     |
| Average                | 82.2                             | 82.9     | 77.7 | 79.2                               | -    | 86.5     | 82.1 | 83.3     |

Table 2: The results on GLUE benchmark. All base models are pre-trained by this work. Every result of the dev set is the average score of 4 times finetuning with different random seeds. Scores of BERT large dev are from (Sun et al., 2019) and scores of BERT large test are from (Devlin et al., 2018).

| System                    | Dev  |            |  |
|---------------------------|------|------------|--|
| o y stelli                | EM   | <b>F</b> 1 |  |
| BERT base (Single)        | 80.8 | 88.5       |  |
| BERT large (Single        | 84.1 | 90.9       |  |
| BERT large (Single+DA)    | 84.2 | 91.1       |  |
| KT-NET                    | 85.2 | 91.7       |  |
| StructBERT Large (Single) | 85.2 | 92.0       |  |
| SegaBERT base (Single)    | 83.2 | 90.2       |  |
| SegaBERT large (Single)   | 85.3 | 92.4       |  |

Table 3: Evaluation results of SQUAD v1.1.

| System           | Dev  |      |  |  |
|------------------|------|------|--|--|
| bystein          | EM   | F1   |  |  |
| BERT base        | 72.3 | 75.6 |  |  |
| BERT base (ours) | 75.4 | 78.2 |  |  |
| SegaBERT base    | 76.3 | 79.2 |  |  |
| BERT large       | 78.7 | 81.9 |  |  |
| BERT large wwm   | 80.6 | 83.4 |  |  |
| SegaBERT large   | 81.8 | 85.2 |  |  |

Table 4: Evaluation results of SQUAD v2.0.

 $F1 = 2 (P^*R) / (P+R)$ , P is precision, R is recall, all in percentage, EM – exact match

| Model  | #Param. | PPL  |
|--|---------|------|
| LSTM+Neural cache (Grave et al., 2017)             | -       | 40.8 |
| Hebbian+Cache (Rae et al., 2018)                   | -       | 29.9 |
| Transformer-XL base, M=150 (Dai et al., 2019)      | 151M    | 24.0 |
| Transformer-XL base, M=150 (ours)                  | 151M    | 24.4 |
| SegaTransformer-XL base, M=150                     | 151M    | 22.5 |
| Adaptive Input (Baevski and Auli, 2019)            | 247M    | 18.7 |
| Transformer-XL large, M=384 (Dai et al., 2019)     | 257M    | 18.3 |
| Compressive Transformer, M=1024 (Rae et al., 2020) | 257M    | 17.1 |
| SegaTransformer-XL large, M=384                    | 257M    | 17.1 |

Table 1: Comparison with Transformer-XL and competitive baseline results on WikiText-103.



(a) SegaBERT-Layer 1

(b) BERT-Layer 1

- 0.040

- 0.035

- 0.030

- 0.025

- 0.020

-0.015

- 0.010

- 0.005

#### (a) SegaBERT-Layer 6





(b) BERT-Layer 6

## **Feature Extraction**



The output of each encoder layer along each token's path can be used as a feature representing that token.



We end up with some embedding for each word related to current input

We start with independent word embedding at first level

But which one should we use?

### Feature Extraction, which embedding to use?

#### What is the best contextualized embedding for "Help" in that context?

For named-entity recognition task CoNLL-2003 NER

Dev F1 Score



## What we have learned

- 1. Model size matters (345 million parameters is better than 110 million parameters).
- 2. With enough training data, more training steps imply higher accuracy
- 3. Key innovation: Learning from unannotated data.

#### Literature & Resources for Transformers

Resources:

OpenAI GPT-2 implementation: <u>https://github.com/openai/gpt-2</u> BERT paper: J. Devlin et al, BERT, pretraining of deep bidirectional transformers for language understanding. Oct. 2018. ELMo paper: M. Peters, et al, Deep contextualized word representation, 2018 ULM-FiT paper: Universal language model fine-tuning for text classification. J. Howeard, S. Ruder., 2018 Jay Alammar, The illustrated GPT-2, <u>https://jalammar.github.io/illustrated-</u>

gpt2/

- T-SNE Worked Example 19.2 T-SNE on MNIST Data
- Generate word embeddings with BOW for spam classification