CS310 Natural Language Processing
自然语言处理
Lecture 08 - Pretraining

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Overview

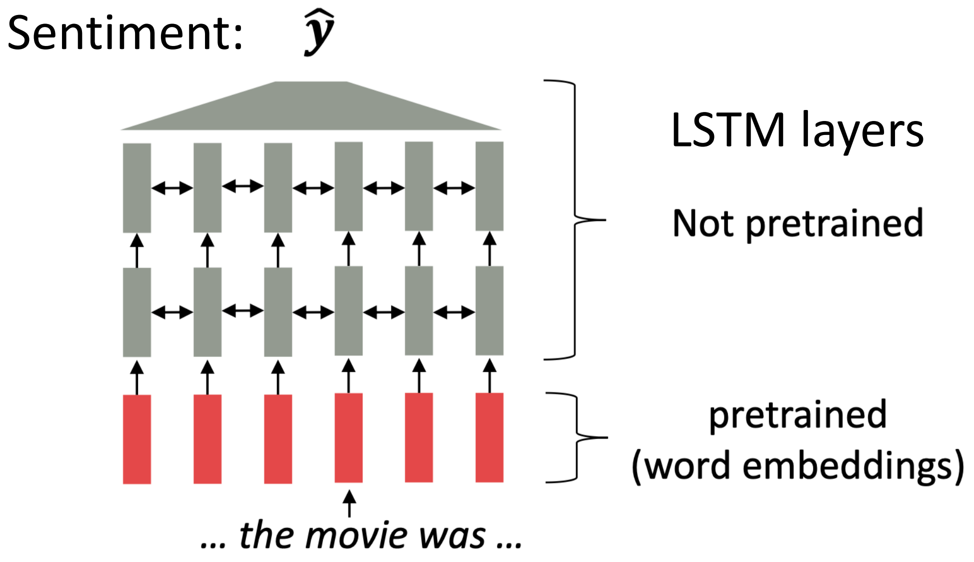
- Architecture
- Tokenization
- Pretraining
- Fine-Tuning
- Contextual Embedding and Word Sense

Overview

- **Architecture**
  - **Autoregressive decoder: GPT**
  - **Autoencoding: BERT**
  - **Encoder-decoder: T5**
  - **General language modeling (GLM)**
- Tokenization
- Pretraining
- Fine-Tuning
- Contextual Embedding and Word Sense

Background

- "pre-" means "before"
- Pretraining: train the model before applying it to a specific task
- Around 2017, state-of-the-art NLP = pretrained word embedding + LSTMs

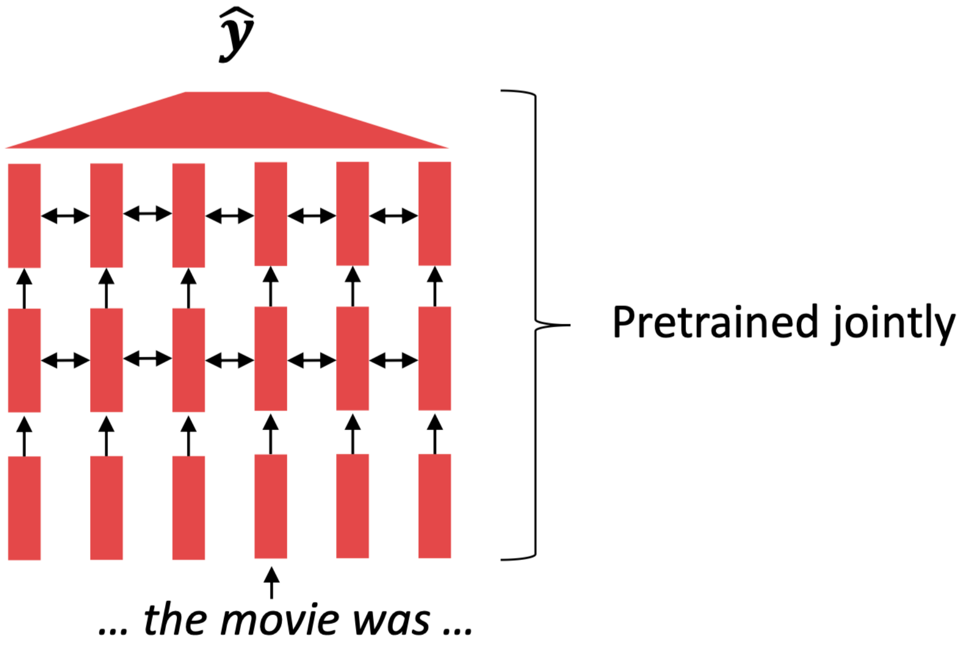


Issues:

- The training data must be sufficient to cover broad aspects of language
- Most params are randomly initialized
- Word representations are not contextualized:
  Ex. "movie" has fixed meaning no matter which sentence it appears in

figure from: https://web.stanford.edu/class/archive/cs/cs224n/cs224n.1224/

Pretraining the whole models



Ex. “movie” has dynamic meaning decided by its context

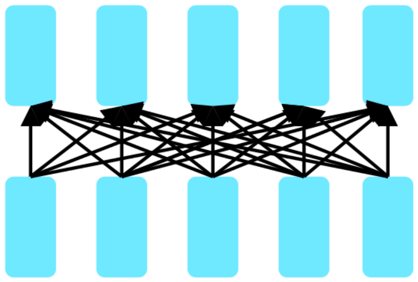
In modern NLP, especially since 2018, **all (or almost all) parameters** are initialized via pretraining

Pretraining:

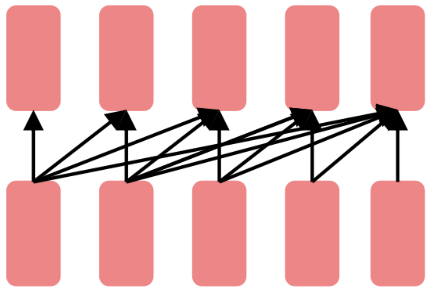
- Better contextualized representations of language
- “Warm up” model params with better initialization
- Make use of large text data

Architecture

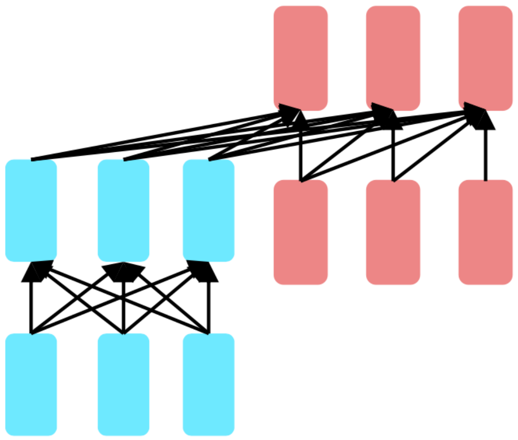
- “Pretraining” can apply to all three types of neural architecture



Encoders



Decoders



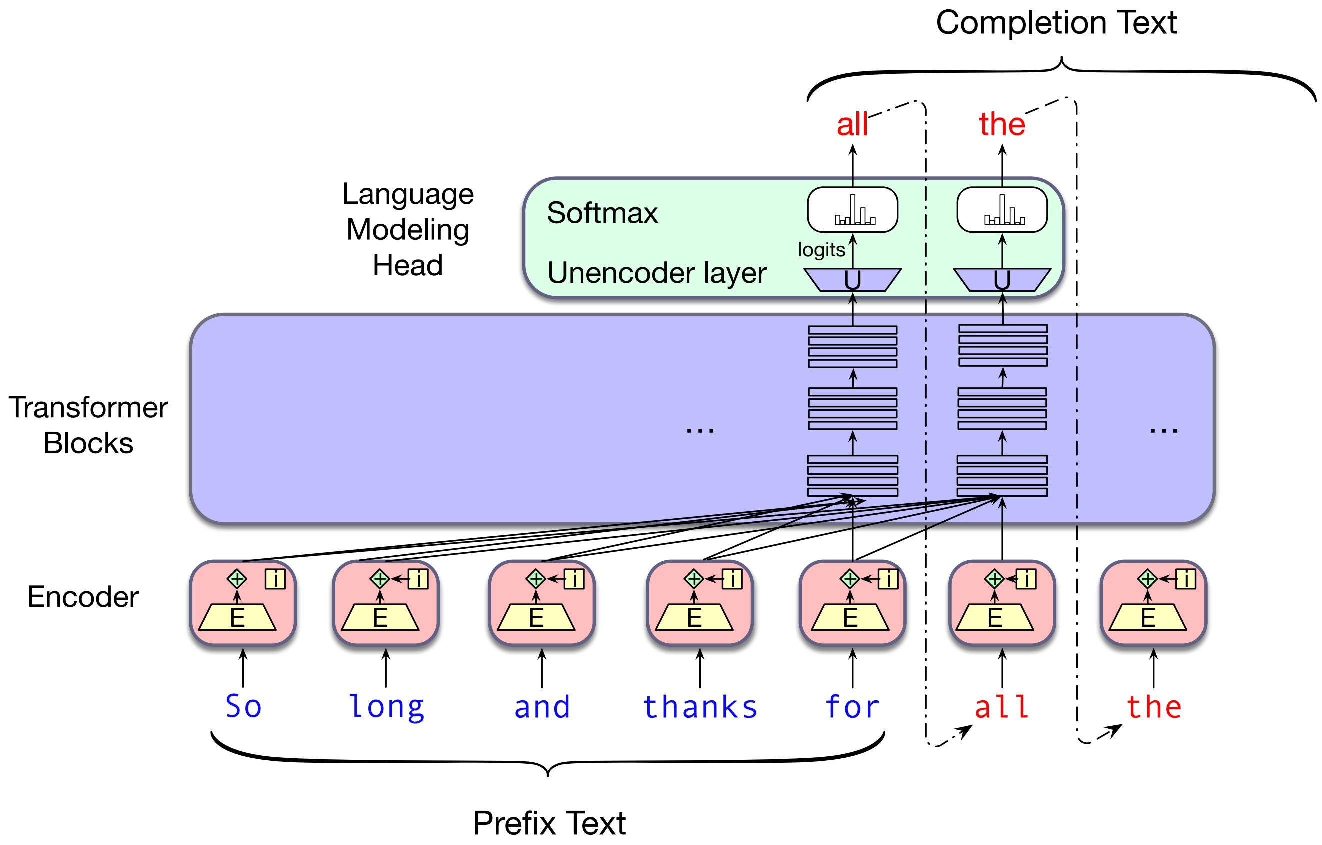
Encoder-decoders

Primary cases

自回归

Autoregressive

- Autoregressive = causal = left-to-right = decoder-only

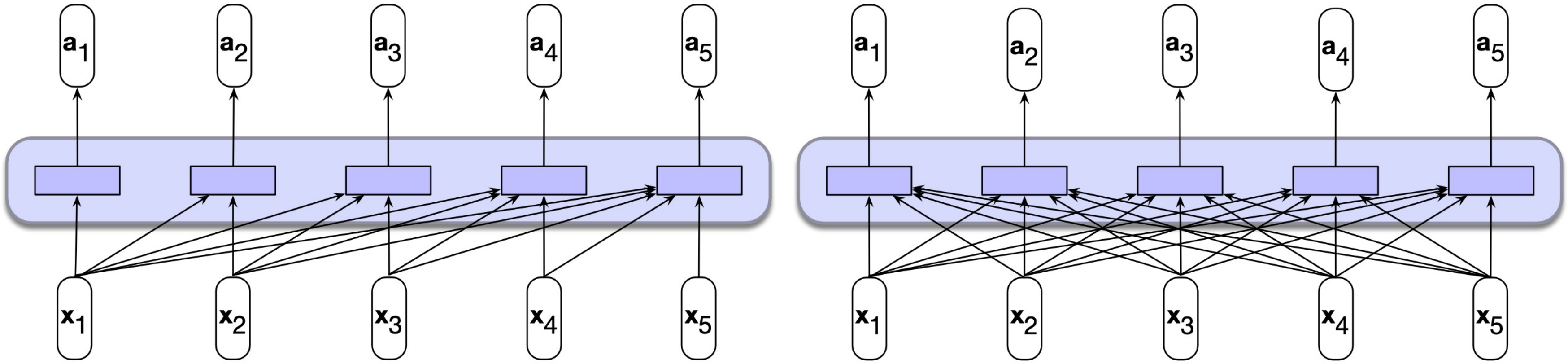


- The model can only see the preceding context
- Ignoring information from the right context

Encoder Model

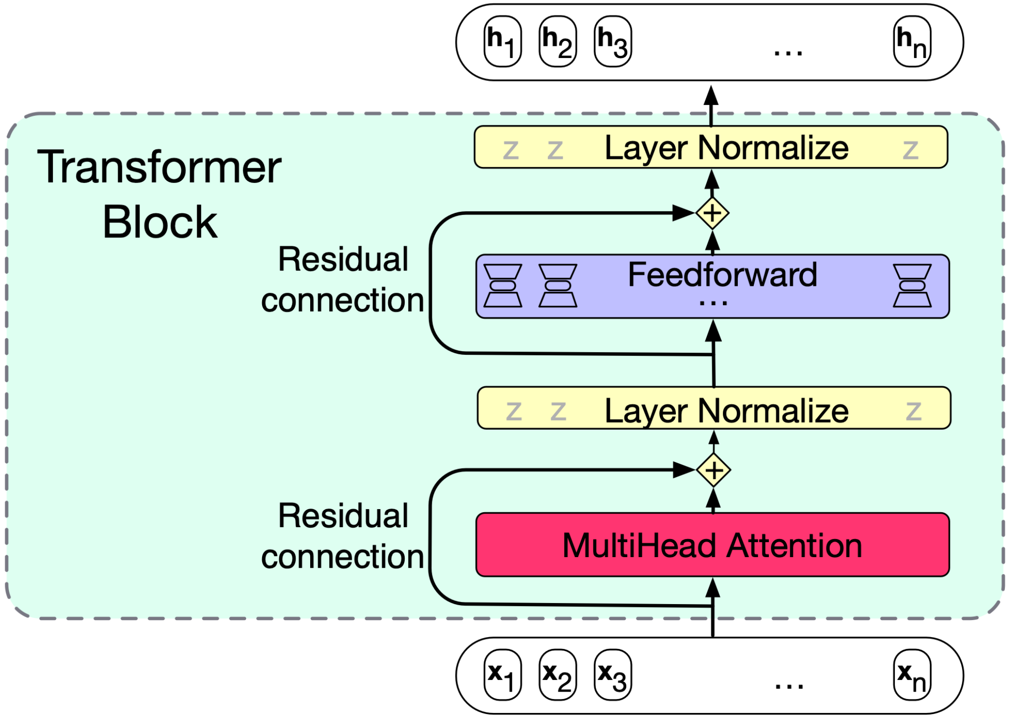
- Bidirectional Encoder Representations from Transformers (**BERT**) (Devlin et al., 2018)
- Its variants: **RoBERTa** (Liu et al., 2019), **ALBERT** (Lan et al., 2019) etc.

- Bidirectional encoders overcome this limitation by allowing self-attention to range over the entire input



a) A causal self-attention layer
b) A bidirectional self-attention layer

BERT Architecture



Uses the same self-attention as causal transformer

$$\boldsymbol{Q}_i = \boldsymbol{X}\boldsymbol{W}_i^Q$$
$$\boldsymbol{K}_i = \boldsymbol{X}\boldsymbol{W}_i^K$$
$$\boldsymbol{V}_i = \boldsymbol{X}\boldsymbol{W}_i^V$$

$$\mathbf{head}_i = \mathrm{SelfAttention}(\boldsymbol{Q}_i, \boldsymbol{K}_i, \boldsymbol{V}_i)$$

$$\boldsymbol{A} = \mathrm{MultiheadAttention}(\boldsymbol{X}) = (\mathbf{head}_1 \oplus \mathbf{head}_2 \ldots \oplus \mathbf{head}_h)\boldsymbol{W}^O$$

$$\mathrm{SelfAttention}(Q, K, V) = \mathrm{softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top}{\sqrt{d_k}}\right)\boldsymbol{V}$$

No future mask is used!

BERT: No Future Mask Used

q1•k1	q1•k2	q1•k3	q1•k4	q1•k5
q2•k1	q2•k2	q2•k3	q2•k4	q2•k5
q3•k1	q3•k2	q3•k3	q3•k4	q3•k5
q4•k1	q4•k2	q4•k3	q4•k4	q4•k5
q5•k1	q5•k2	q5•k3	q5•k4	q5•k5

N

N

The $QK^\top$ matrix contains **all pairs** of comparison between input queries and keys

allowing the model to contextualize each token using *information from the entire input*

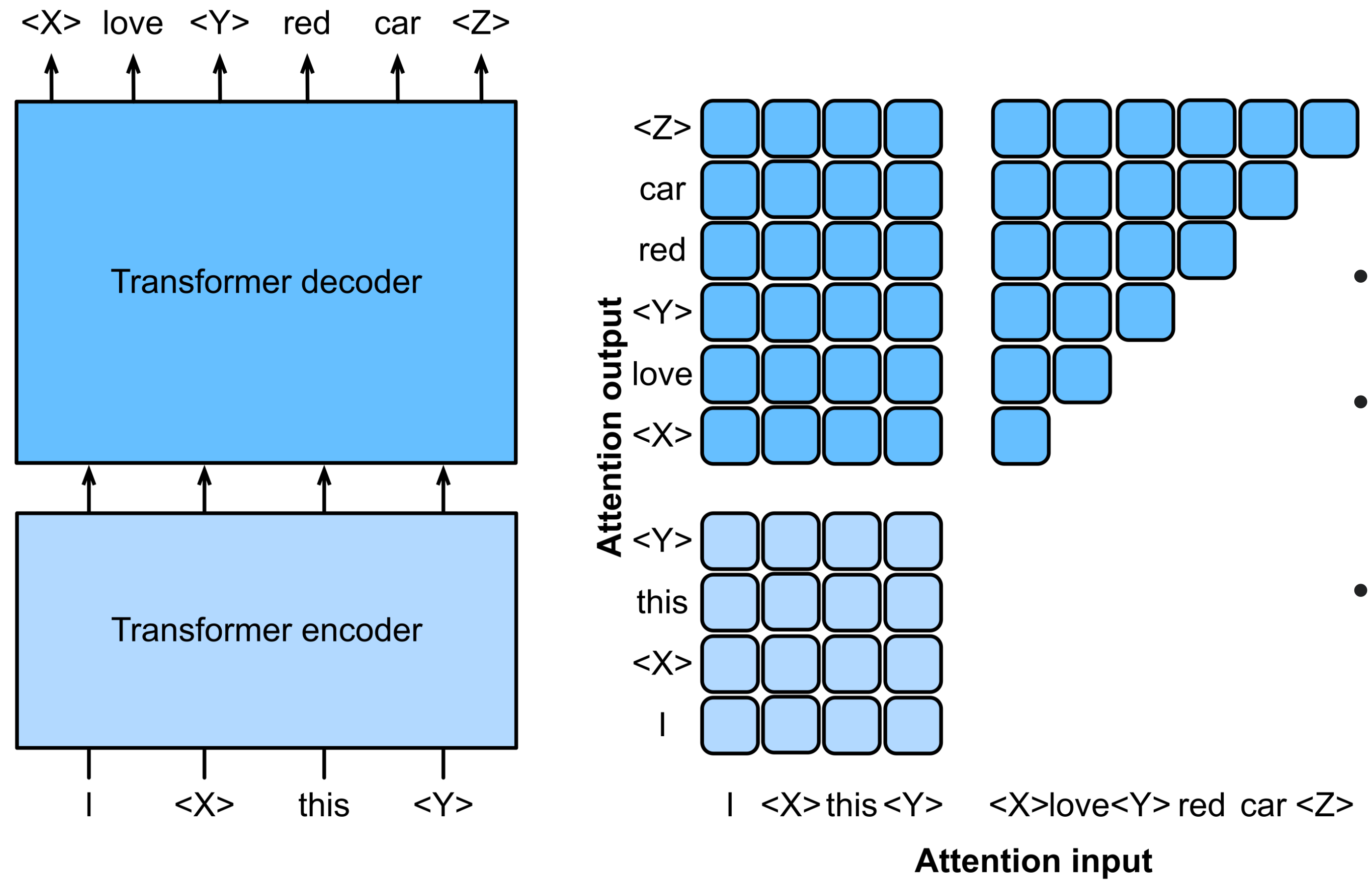
BERT: Hyper Parameters

- **BERT** (Devlin et al., 2018)
- Vocabulary size: 30,000 tokens (from WordPiece algorithm)
- Hidden layer size $d = 768$
- 12 layers of transformer blocks, with 12 multihead attention layers each
- Total params: about **100 M**

- **XLM-RoBERTa** (Liu et al., 2019)
- Vocabulary size: 250,000 tokens (from SentencePiece Unigram LM algorithm)
- Hidden layer size $d = 1024$; 24 layers of transformer blocks, with 16 multihead attention layers each
- Total params: about **550 M**

Encoder-Decoder Model

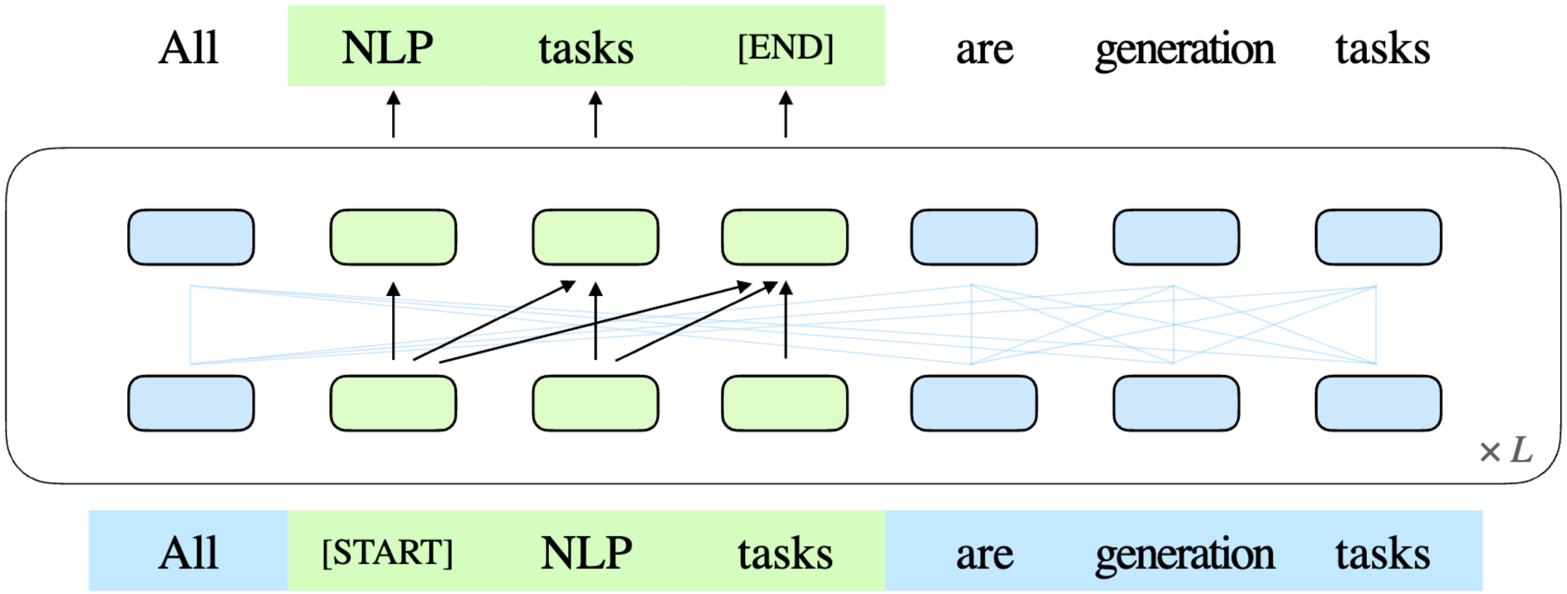
- T5 (Google, 2019)



- Encoder self-attention (lower square), all input tokens attend to each other;
- Encoder–decoder cross-attention (upper rectangle), each target token attends to all input tokens
- Decoder self-attention (upper triangle), each target token attends to present and past target tokens only

General language modeling (GLM) Du et al., 2022

- GLM: Randomly blank out spans of tokens and train the model to sequentially reconstruct the spans.



GLM

Du et al., 2022

$x_1 \quad x_2 \quad x_3 \quad x_4 \quad x_5 \quad x_6$

(a) Sample spans from the input text

The original text is $[x_1, x_2, x_3, x_4, x_5, x_6]$.
Two spans $[x_3]$ and $[x_5, x_6]$ are sampled.

Part A: $x_1 \quad x_2 \quad [\mathrm{M}] \quad x_4 \quad [\mathrm{M}]$

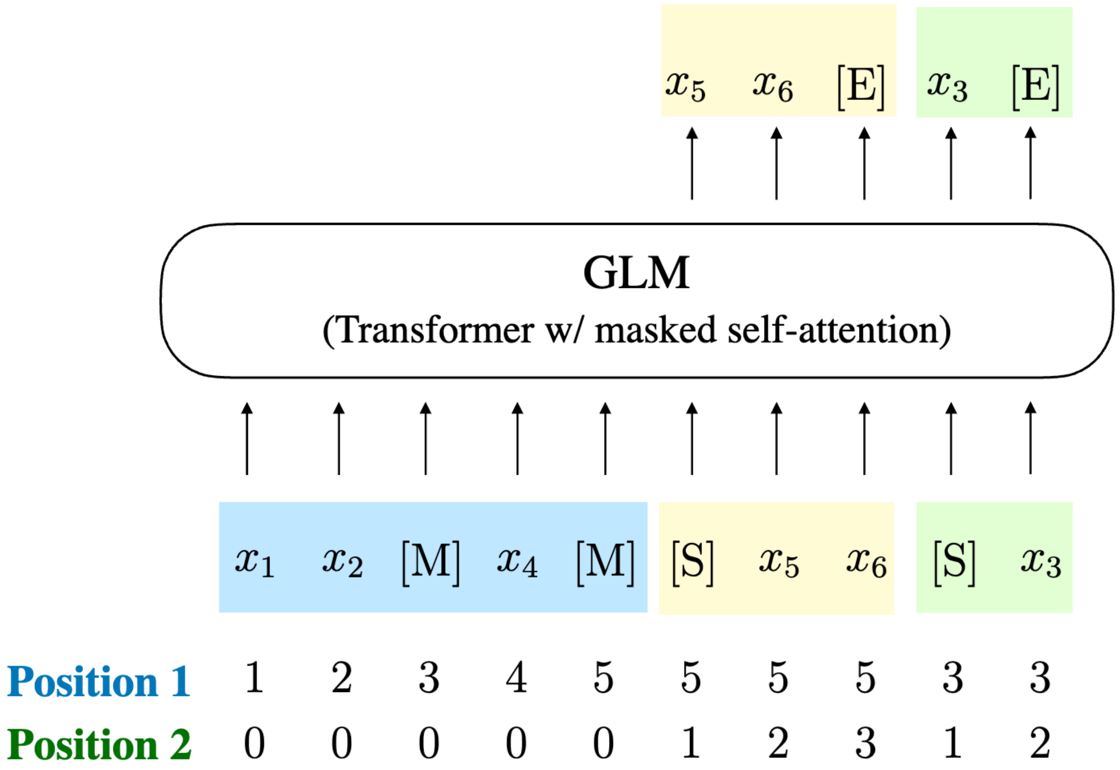
Part B: $x_3 \qquad x_5 \quad x_6$

(b) Divide the input into Part A / Part B

Replace the sampled spans with [M] in Part A, and shuffle the spans in Part B

GLM

Du et al., 2022



(c) Generate the Part B spans autoregressively

Overview

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General tokenization workflow

(input)	Hello how are U tday?
Normalization	hello how are u tday?
Pre-tokenization	[hello, how, are, u, tday, ?]
Model	[hello, how, are, u, td, ##ay, ?]
Postprocessor	[CLS, hello, how, are, u, td, ##ay, ?, SEP]

Here "model" means a **tokenizer model**

Example: `tday => td, ##ay`

Figure source: https://huggingface.co/learn/llm-course/en/chapter6/4?fw=pt

Why subword is necessary

- Weakness of word-level tokenization:
- All *novel* words are mapped to UNK at testing time

	word		vocab mapping
Common words	hat	→	pizza (index)
	learn	→	tasty (index)
Variations	taaaaasty	→	UNK (index)
misspellings	laern	→	UNK (index)
novel items	Transformerify	→	UNK (index)

Subword-Level Tokenization

- Subword tokenization learns a vocabulary of subword tokens
- Split each word into a sequence of known subwords, for both training and testing

	word		vocab mapping
Common words	hat	→	hat
	learn	→	learn
Variations	taaaaasty	→	taa## aaa## sty
misspellings	laern	→	la## ern##
novel items	Transformerify	→	Transformer## ify

The hashtag "#" usage is from the WordPiece tokenization algorithm used in BERT

Byte-Pair Encoding (BPE) Tokenization

- A “bottom-up” algorithm: building the vocabulary by incrementally merging the most frequent pairs

Example corpus:

```
"hug", "pug", "pun", "bun", "hugs"
```

Initial vocabulary:

```
["b", "g", "h", "n", "p", "s", "u"]
```

with frequency:

```
("hug", 10), ("pug", 5), ("pun", 12), ("bun", 4), ("hugs", 5)
```

Example credits to: https://huggingface.co/learn/llm-course/en/chapter6/5?fw=pt

BPE Tokenization cont.

- Splitting each word into characters

```
("h" "u" "g", 10), ("p" "u" "g", 5), ("p" "u" "n", 12), ("b" "u" "n", 4), ("h" "u" "g" "s", 5)
```

Look at **pairs**, and **merge** the most frequent one: `("u", "g") -> "ug"`

```
Vocabulary: ["b", "g", "h", "n", "p", "s", "u", "ug"]
Corpus: ("h" "ug", 10), ("p" "ug", 5), ("p" "u" "n", 12), ("b" "u" "n", 4), ("h" "ug" "s", 5)
```

BPE Tokenization cont.

- Given the new corpus, merge the next most frequent pair `("u", "n") -> "un"`

```
Vocabulary: ["b", "g", "h", "n", "p", "s", "u", "ug", "un"]
Corpus: ("h" "ug", 10), ("p" "ug", 5), ("p" "un", 12), ("b" "un", 4), ("h" "ug" "s", 5)
```

- Next `("h", "ug") -> "hug"`

```
Vocabulary: ["b", "g", "h", "n", "p", "s", "u", "ug", "un", "hug"]
Corpus: ("hug", 10), ("p" "ug", 5), ("p" "un", 12), ("b" "un", 4), ("hug" "s", 5)
```

- …
- repeat until a desired vocabulary size is reached

Deal with Unicode characters

- GPT-2, RoBERTa, and recent Qwen, DeepSeek series use **Byte-level BPE**
- Process words not with Unicode characters, but with bytes
- Every character (Chinese, Japanese, Korean, emoji, …) will be included, but not end up being unknown tokens

Overview

- Architecture
- Tokenization
- **Pretraining Task**
  - **Token level: Masked Language Models**
  - **Sequence level: Next Sentence Prediction**
  - **Training Method**
- Fine-Tuning
- Contextual Embedding and Word Sense

Pretraining of Bidirectional Encoders

- A new training scheme other than next-word-prediction:
- **Fill-in-Blank task** -- **close task**
- Predict a missing item given the rest of the sentence

```
Please turn _____ homework in
```

- instead of predicting the next word

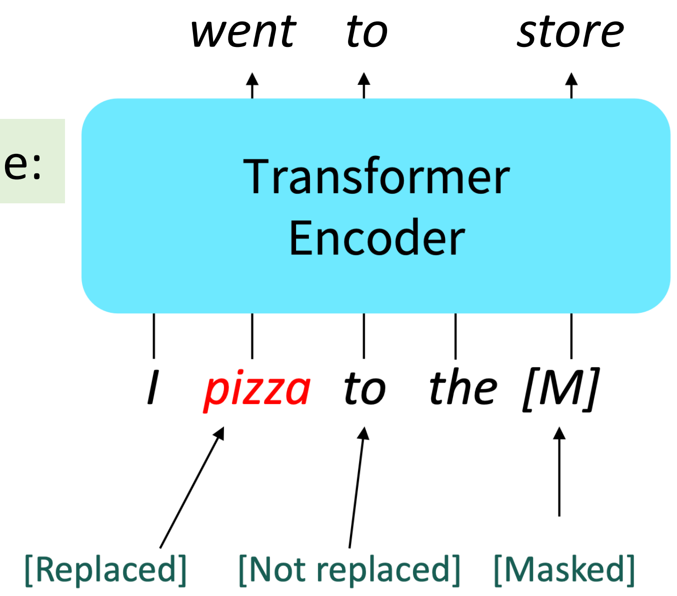
```
Please turn your homework _______
```

Masked Language Modeling

- The original approach used in BERT: Masked Language Modeling (MLM)
- **Randomly sample 15%** of the input tokens from each training sentence
- Among these sampled tokens:
- ⇒ 80% are replaced with a special token **[MASK]**
- ⇒ 10% are replaced with another randomly selected token
- ⇒ 10% are left unchanged
- Why? Prevent the model from getting complacent and not building strong representations of non-masked words
- All tokens play a role in self-attention process, but only the sampled tokens are used for learning

Example:

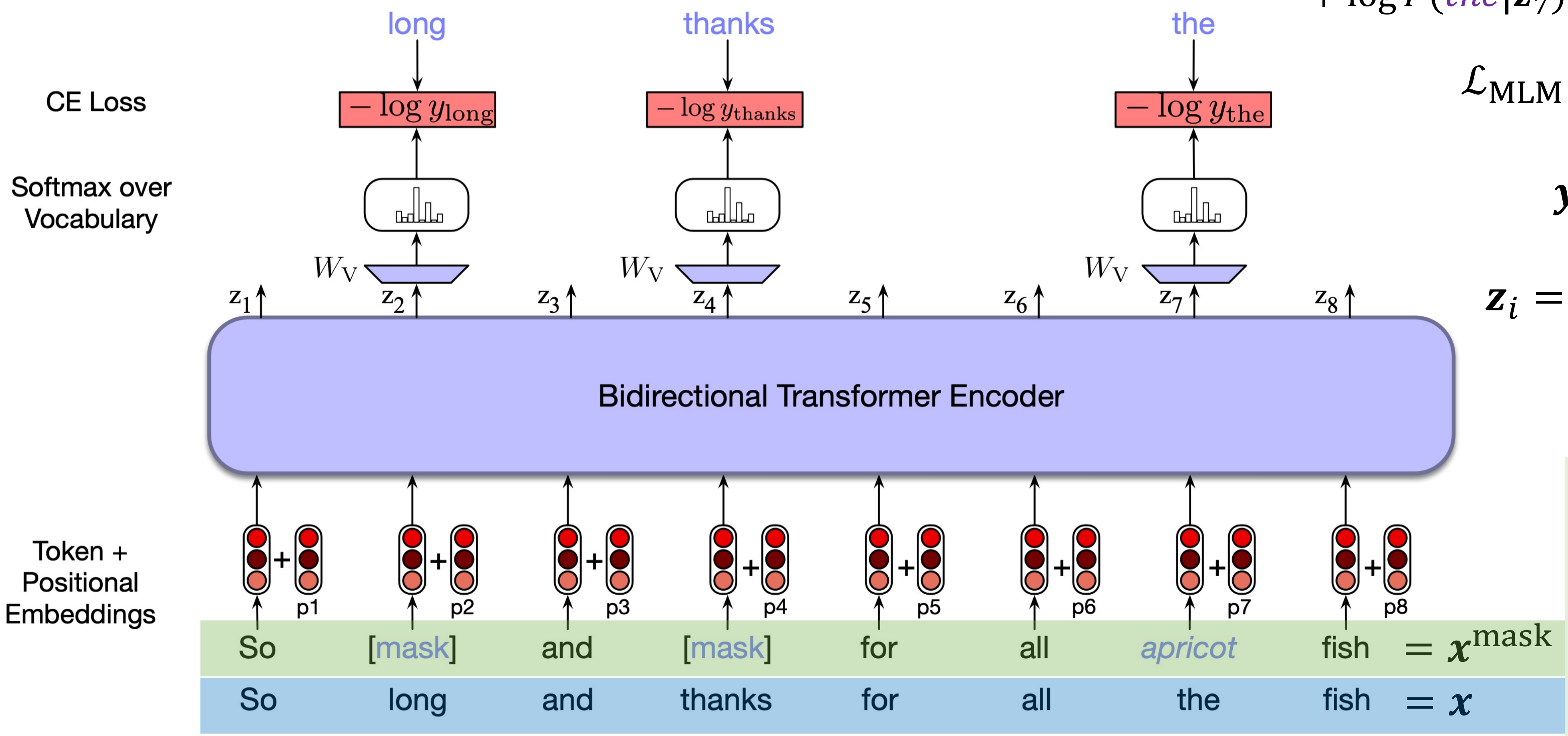
Original sentence:
I went to the store



MLM Overview

$$\mathcal{L}_{\text{MLM}} = -\frac{1}{|M|}\sum_{i\in M}\log P(x_i|\boldsymbol{z}_i)$$

$$= -\frac{1}{3}\left(\log P(\textit{long}|\boldsymbol{z}_2) + \log P(\textit{thanks}|\boldsymbol{z}_4) + \log P(\textit{the}|\boldsymbol{z}_7)\right)$$



$$\mathcal{L}_{\text{MLM}}(x_i) = -\log P(x_i|\boldsymbol{z}_i)$$

$$\boldsymbol{y}_i = \text{softmax}(\boldsymbol{W}_V\boldsymbol{z}_i)$$

$$\boldsymbol{z}_i = \text{TransformerEnc}(\boldsymbol{x}^{\text{mask}})$$

$$\boldsymbol{z}_i \in \mathbb{R}^d$$

The masked tokens $M = \{\textit{long}, \textit{thanks}, \textit{the}\}$ have been sampled:

long ⇒ [MASK]

thanks ⇒ [MASK]

the ⇒ *apricot*

MLM Notes

- Only 15% of the input data are used for training
- Because on the sampled tokens in M play a role in the loss $\mathcal{L}_{MLM} = -\frac{1}{|M|}\sum_{i \in M} \log P(x_i | \boldsymbol{z}_i)$
- Other tokens play no role
- Thus, training BERT with MLM is inefficient
- Some members of BERT family use all examples for training, e.g., ELECTRA (Clark et al., 2020)

Next Sentence Prediction

- Some NLP applications involves determining the relationship between pairs of sentences, such as:
- **Paraphrase (改述)** detection: if two sentences have similar meanings
- **Entailment (蕴含)**: detect if s_1 entails s_2, or contradict
- **Discourse coherence** (话语连贯性): detect if two neighboring sentences form a coherent discourse

Paraphrase
- s1: "这个苹果很甜。" (This apple is very sweet.)
- s2: "这个苹果味道很好。" (This apple tastes really good.)

Entailment
- Premise: "The sky is blue."
- Hypothesis: "The sky is a shade of azure."

In this example, the hypothesis logically follows from the premise, indicating entailment.

Discourse coherence
"我想要一杯咖啡。狗在睡觉。" (I want a cup of coffee. The dog is sleeping.)
This is an negative example

Next Sentence Prediction

- Presented with pairs of sentences, the model's task is to predict whether each pair is an **ACTUAL** pair of adjacent sentences from the training corpus, or a pair of randomly sampled unrelated sentences
- BERT uses 50% of sentences in true pairs, and the other 50% random pairs
- Two new tokens to facilitate training:
- **[CLS]**: prepended to input pair s_1, s_2 ("CLS" for "classification")
- **[SEP]**: placed between s_1 and s_2, and after s_2
- Finally, add extra embeddings to distinguish s_1 and s_2

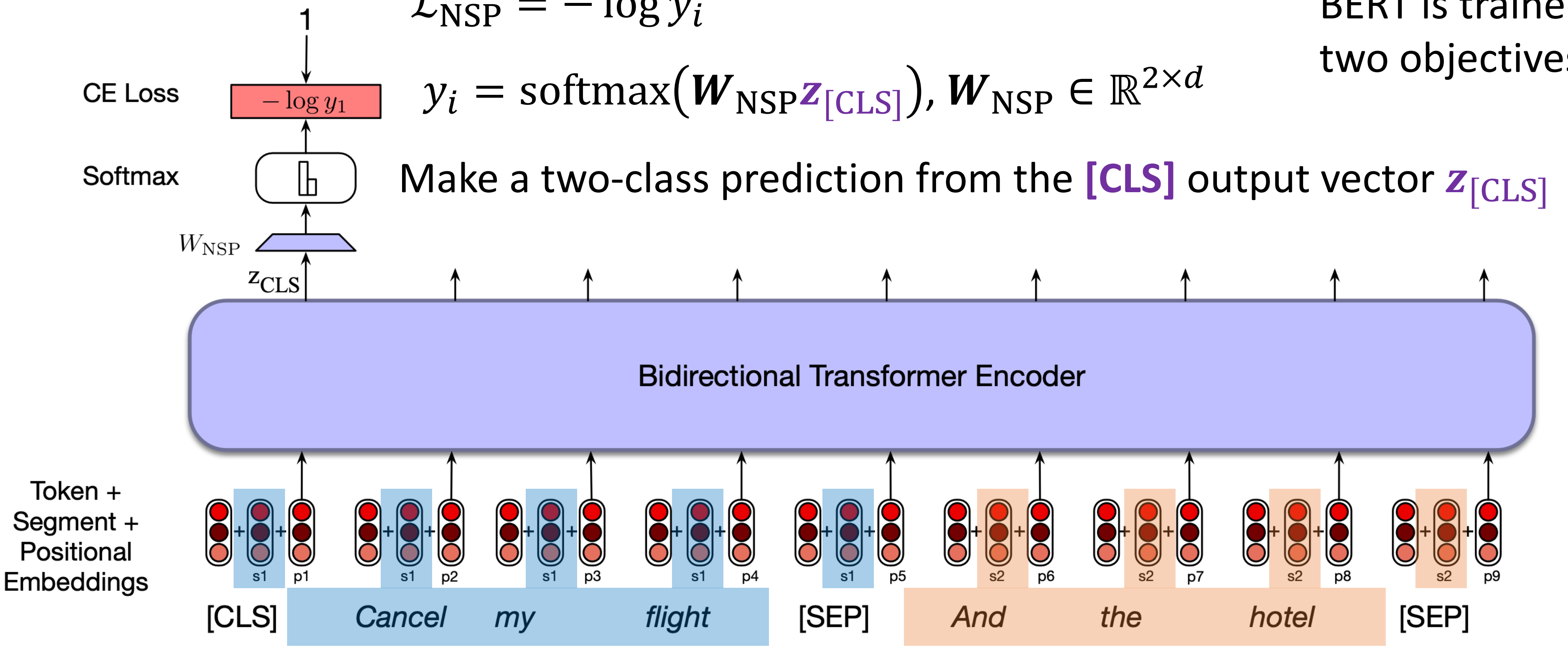
Next Sentence Prediction

$$\mathcal{L}_{\mathrm{NSP}} = -\log y_i$$

$$y_i = \mathrm{softmax}(\boldsymbol{W}_{\mathrm{NSP}} \boldsymbol{z}_{[\mathrm{CLS}]}),\ \boldsymbol{W}_{\mathrm{NSP}} \in \mathbb{R}^{2\times d}$$

Make a two-class prediction from the **[CLS]** output vector $\boldsymbol{z}_{[\mathrm{CLS}]}$

BERT is trained by combining the two objectives: $\mathcal{L}_{\mathrm{MLM}} + \mathcal{L}_{\mathrm{NSP}}$



Sentence 1 with extra embedding s_1

Sentence 2 with extra embedding s_2

Training Details of BERT

- Two models released (Devlin et al., 2018)
  - BERT-base: 12 layers (transformer blocks), 768-dim, 12 attention heads, 110 million params
  - BERT-large: 24 layers, 1024-dim, 16 attention heads, 340 million params
- Training data
  - BooksCorpus (800 million words)
  - English Wikipedia (2,500 million words)
- Trained on 64 TPUs for 4 days
  - Pretraining is impractical on a single GPU
- Yet, fine-tuning is practical and common on a single GPU
  - “Pretrain once, fine-tune many times”

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- **Fine-Tuning**
- Contextual Embedding and Word Sense

Fine-Tuning

- **Fine-tuning**: add a small set of application-specific parameters on top of pretrained models
- Use ***labeled data*** to train these application-specific parameters
- Either ***freeze*** or make only ***minimal*** adjustments to the pretrained parameters
- Common applications:
    - Sequence classification
    - Pair-Wise sequence classification
    - Sequence labeling
    - Span-based operations (more advanced)

Sequence Classification

- An input sequence is represented with a single consolidated representation
- Recall RNN: use the final hidden state to stand for the entire sequence
- In transformer-based model: use an additional **vector** to represent the entire sequence ⇒ sometimes called **sentence embedding**

- In BERT, use the output vector of **[CLS]** , $\boldsymbol{z}_{[\mathrm{CLS}]}$, plays this role
  - [CLS] is added to vocabulary and prepended to all input sequences during pretraining
- $\boldsymbol{z}_{[\mathrm{CLS}]}$ serves as input to a **classifier head** -- a network classifier to make relevant predictions

Sequence Classification

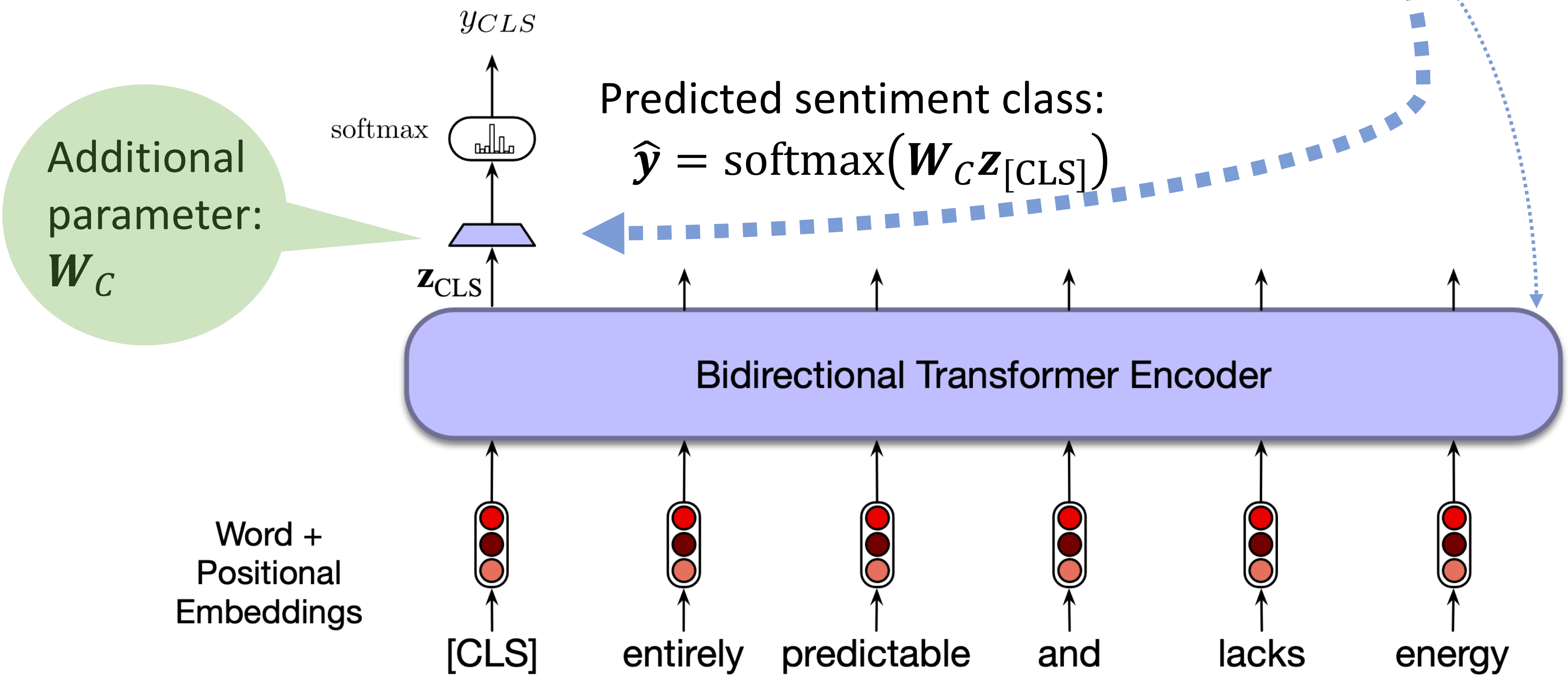
Example: Sentiment classification

Cross-Entropy loss:

$$\mathcal{L}_{\text{CE}} = \text{CrossEntropy}(\hat{\boldsymbol{y}}, \boldsymbol{y}) = -\log \hat{\boldsymbol{y}}$$

Predicted sentiment class:

$$\hat{\boldsymbol{y}} = \text{softmax}\big(\boldsymbol{W}_C \boldsymbol{z}_{[\text{CLS}]}\big)$$



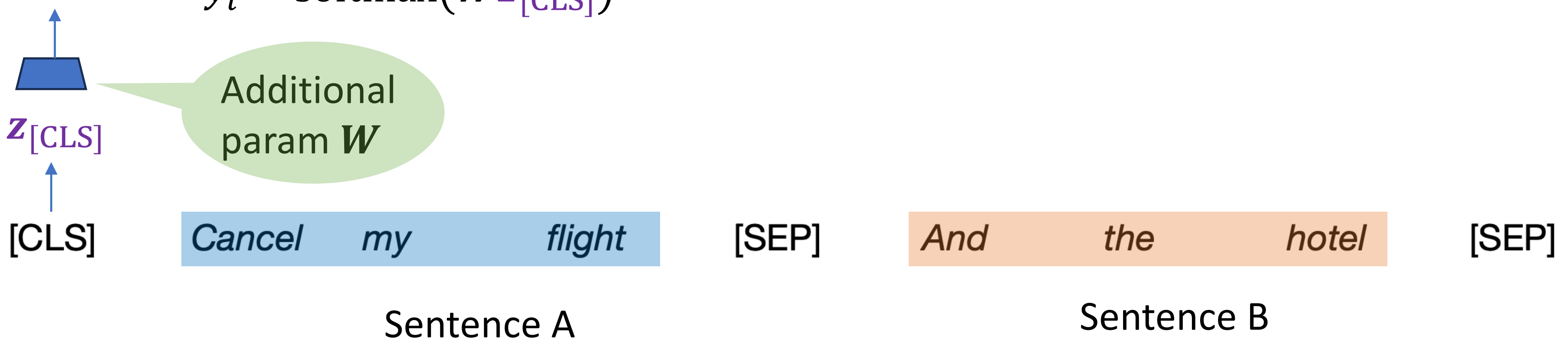
Difference from training a small neural classifier:

- Loss is mainly used to update param $\boldsymbol{W}_C$
- Minimal changes are made to the encoder params: limited to updates over the **final few transformer layers**

Pair-Wise Sequence Classification

- **Paraphrase detection**: are sentence A and B paraphrases of each other?
- **Logical entailment**: does sentence A logically entail sentence B?
- **Discourse coherence**: how coherent is sentence B as a follow-on to sentence A?
- Fine-tuning these tasks proceeds just as with the next sentence prediction (NSP) pretraining task

$$y_i = \text{softmax}(\boldsymbol{W}\boldsymbol{z}_{[\text{CLS}]})$$



Example: entailment classification

- Dataset: Multi-Genre Natural Language Inference (MultiNLI)
- Pairs of sentences mapped to one of 3 labels: {entail, contradicts, neutral}

Entails
a: I'm confused.
b: Not all of it is very clear to me.

Neutral
a: Jon walked back to the town to the smithy.
b: Jon traveled back to his hometown.

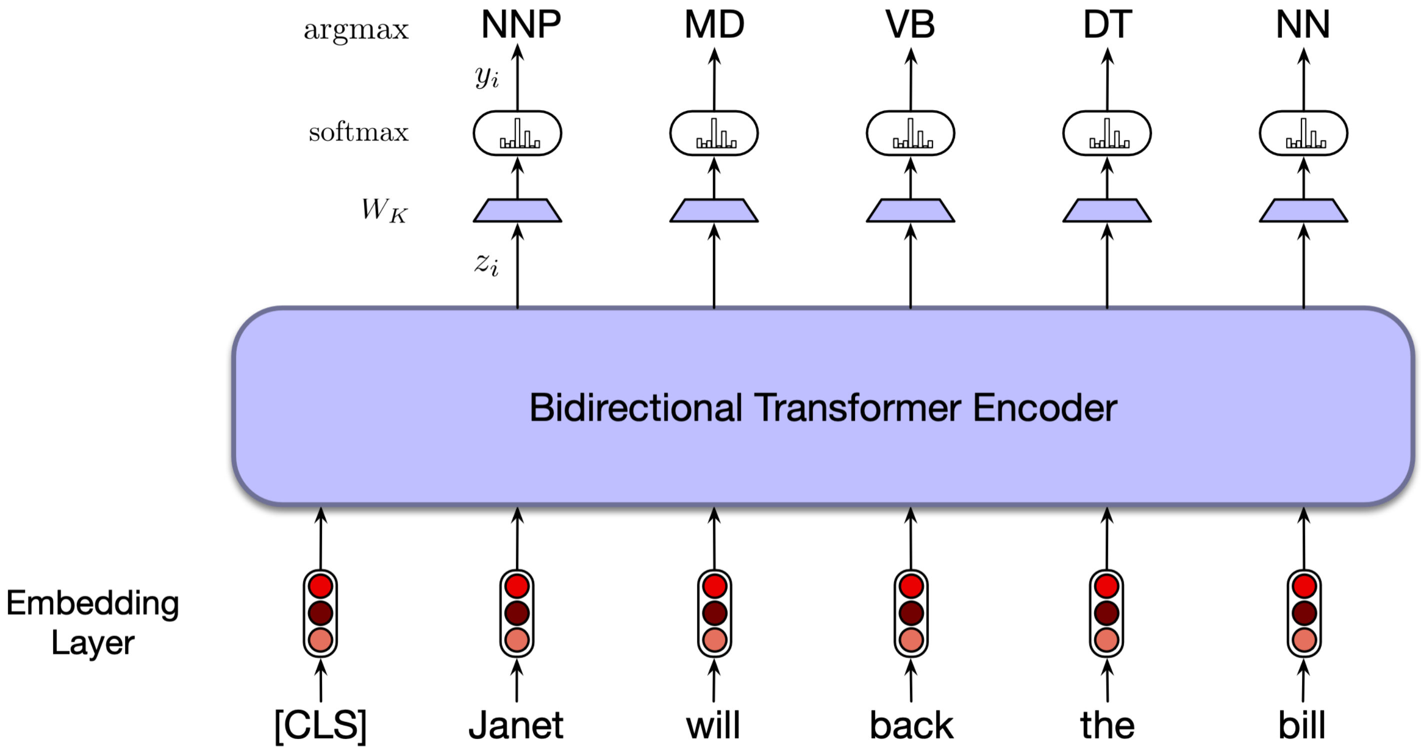
Contradicts
a: Tourist Information offices can be very helpful.
b: Tourist Information offices are never of any help.

$$y_i = \text{softmax}\left(\boldsymbol{W}\boldsymbol{z}_{[\text{CLS}]}\right) \in \mathbb{R}^3$$

(Williams et al., 2018)

Sequence Labeling

- The final output vector z_i corresponding to **each input token** x_i is passed to a classifier to produce a probability distribution over possible labels
- Example: POS tagging, BIO-based NER



Additional param: $W_K \in \mathbb{R}^{k \times d}$ for k possible tags

with greedy approach:

$$\hat{y}_i = \mathrm{softmax}(\boldsymbol{W}_K \boldsymbol{z}_i)$$

$$y_i = \arg\max_k \hat{y}_i$$

More advanced: pass $\hat{y}_i$ to a conditional random field (CRF) layer and use viterbi decoding

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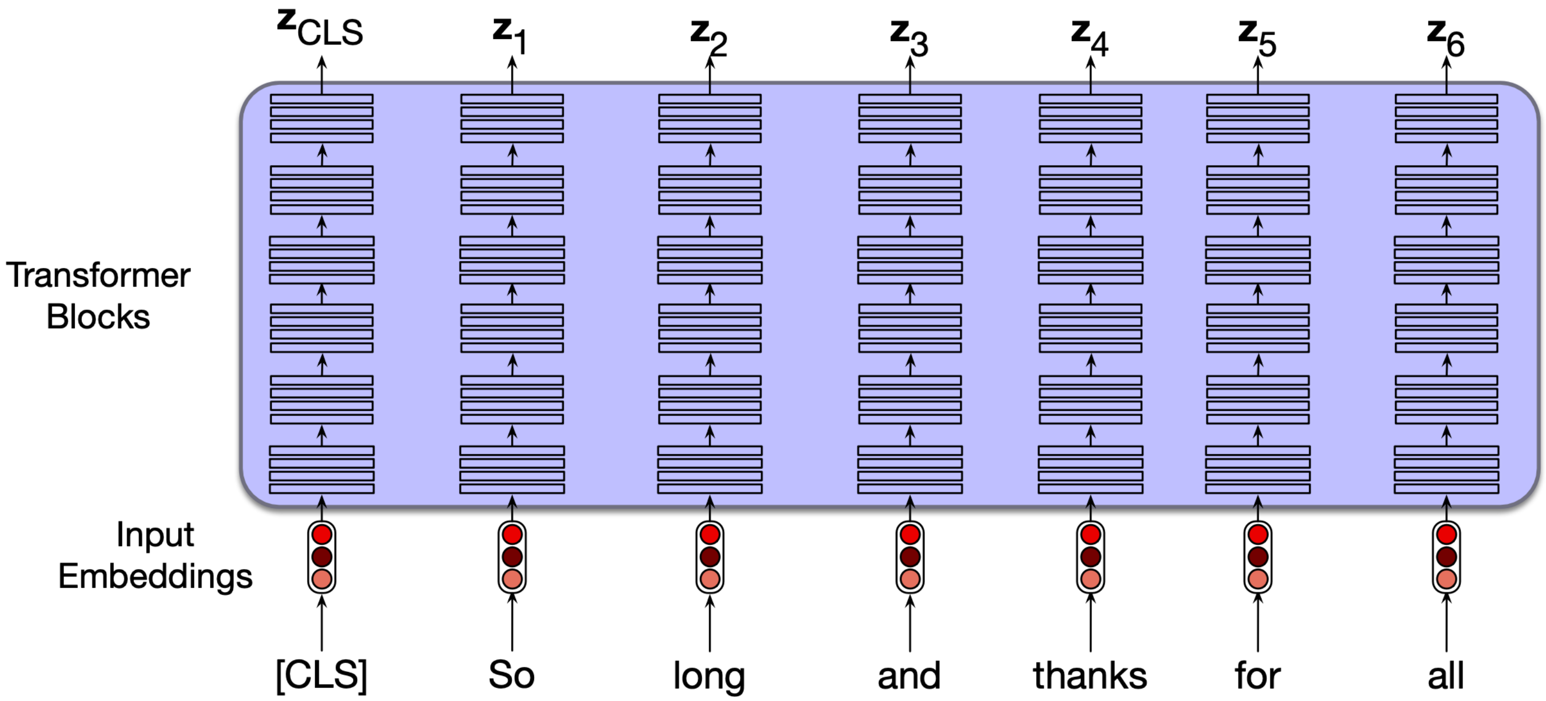
Contextual Embeddings

- The output of a BERT-style model is a contextual embedding vector z_i for each input token x_i
  - z_i represents some aspects of the meanings of x_i
  - Sometimes, instead of just using the final layer, we can average the z_i from the last four layers



Contextual Embeddings

- Static embedding (e.g., word2vec) ⇒ meaning of a word ***types***
  - a type is a static entry in the vocabulary
- Contextual embedding ⇒ meaning of word ***instances***
  - Instances of a particular word type in a particular context
- Thus, contextual embeddings are useful in linguistic tasks that require models of word meaning

- "I would like some orange juice" ⇒ fruit
- "Paint this part orange" ⇒ color

Word Sense

- Words are ambiguous: same word can be used to mean different things
- **Polysemous** (多义词), Geek “many senses”
- A **word sense** is a discrete representation of *one meaning* of a word

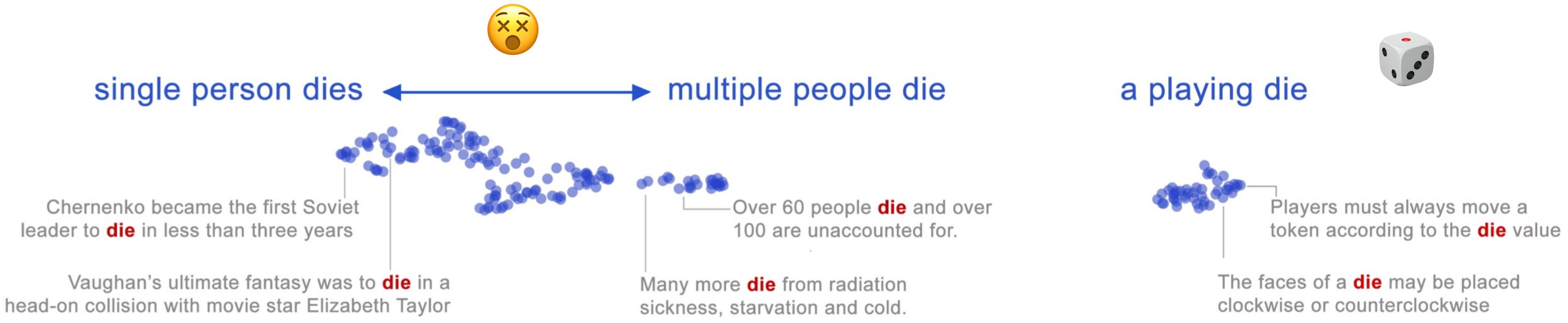
mouse^1 : .... a *mouse* controlling a computer system in 1968.
mouse^2 : .... a quiet animal like a *mouse*
bank^1 : ...a *bank* can hold the investments in a custodial account ...
bank^2 : ...as agriculture burgeons on the east *bank*, the river ...

- The senses can be visualized geometrically by contextual embeddings

Visualize Word Senses

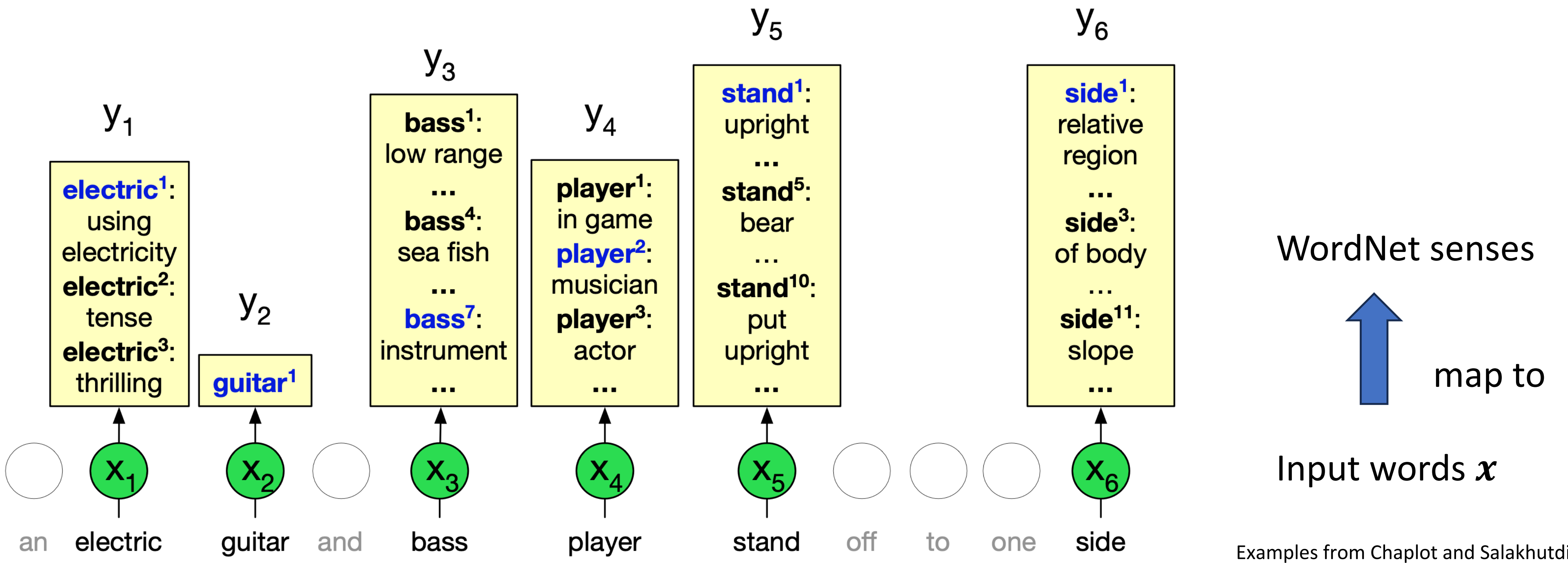
Figure from Coenen et al. (2019)

- Dictionary and thesauruses like WordNet give **discrete** lists of senses
- Embeddings (whether contextual or static) provides a **continuous high-dimensional** view of meaning



Word Sense Disambiguation

- **Word Sense Disambiguation**: the task of selecting the correct sense for a word
- Takes as input a word in context and a fixed inventory of potential word senses (like the ones in WordNet) and outputs the correct sense in context



Examples from Chaplot and Salakhutdinov, 2018

WSD Algorithm: 1-nearest-neighbor

- At training time: pass a sense-labeled dataset through any contextual embedding (e.g., BERT) ⇒ vector v_i for each token i
- For each sense s of any word, and for each of the n tokens of that sense, produce a **sense embedding** $\boldsymbol{v}_s$ by averaging the n contextual embeddings:

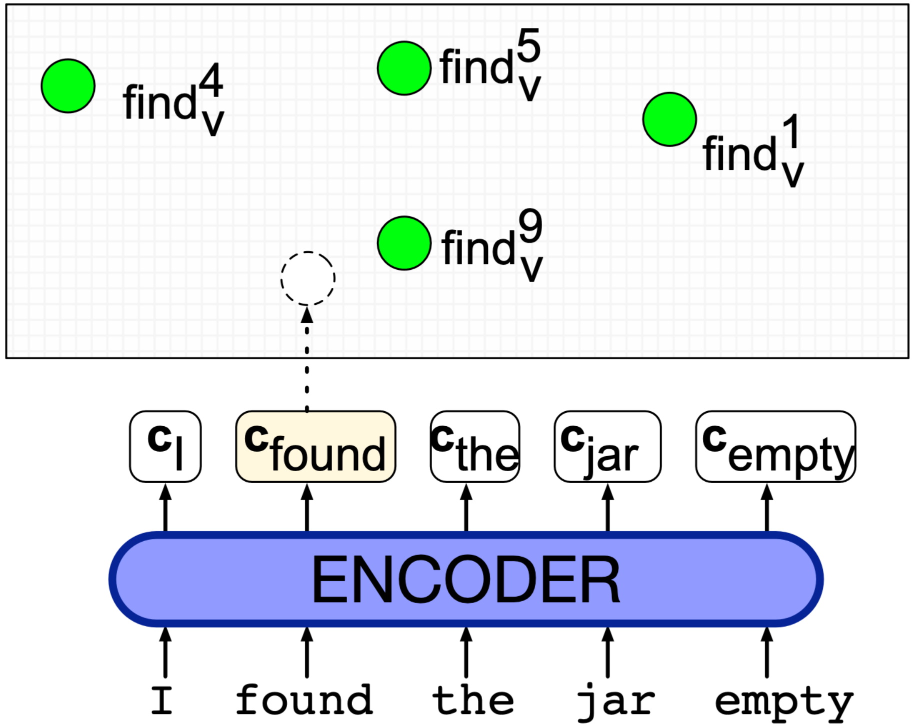
$$\boldsymbol{v}_s = \frac{1}{n}\sum_i v_i \qquad \forall \boldsymbol{v}_i \in \text{tokens}(s)$$

- At test time, given a token of target word t, compute its contextual embedding t and choose its nearest neighbor sense from the training set:

$$\text{sense}(t) = \arg\max_{s\in\text{senses}(t)} \cos(\boldsymbol{t}, \boldsymbol{v}_s)$$

WSD 1-nearest-neighbor Example

- Contextual embedding for *found* c_{found} is computed, and the nearest neighbor sense $\mathbf{find}_v^9$ is chosen



Examples from Loureiro and Jorge, 2019

Word Similarity is Tricky

- **Fact**: Contextual embeddings for all words are *extremely similar*
- **Fact**: BERT embeddings of any two randomly chosen words will have extremely high cosines $\approx 1 \Rightarrow$ All word vectors tend to point in the same direction
- A property known as **anisotropy** (各向异性)
- Anisotropy $\triangleq$ the expected cosine similarity of any pair of words in a corpus (Ethayarajh, 2019)
- If all vectors are uniformly distributed, then the expected cosine should be 0, which we call **isotropy** (各向同性)
- Cause of anisotropy: cosine measures are dominated by a small number of rogue dimensions that have very large magnitudes and high variance (Timkey and van Schijndel, 2021)

Solution to Anisotropy

- Standardizing (z-scoring) the vectors, i.e., subtracting the mean and dividing by variance

$$\mu = \frac{1}{|C|}\sum_{\boldsymbol{x}\in C} \boldsymbol{x} \quad \sigma = \sqrt{\frac{1}{|C|}\sum_{\boldsymbol{x}\in C}(\boldsymbol{x}-\mu)^2} \quad z = \frac{x-\mu}{\sigma}$$

- Remaining problem: cosine tends to underestimate similarity of word meanings for very frequent words (according to human judgements) (Zhou et al., 2022)

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