# Training and Finetuning Transformers. Supervised Learning, Transfer Learning, Few-Shot and Zero-shot learning

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# Outline

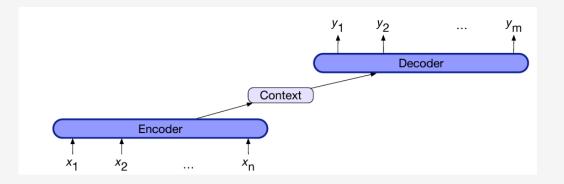
- Quick recap
- The encoder-decoder transformer
  - Training a transformer model
- Transfer Learning and Finetuning
  - Decoder transformers: GPT
  - Encoder transformers: BERT
- In-context learning. Zero-shot and Few-shot learning

# Quick recap: Encoder Decoder. Attention. Transformers.

# Encoder decoder models

- Mapping between data of different format, size, and structure
  - Two texts of different length and alignment, image and text

- Simple idea
  - Encoder "represents" the source (e.g., English)
  - Decoder "generates" the target (e.g., German)



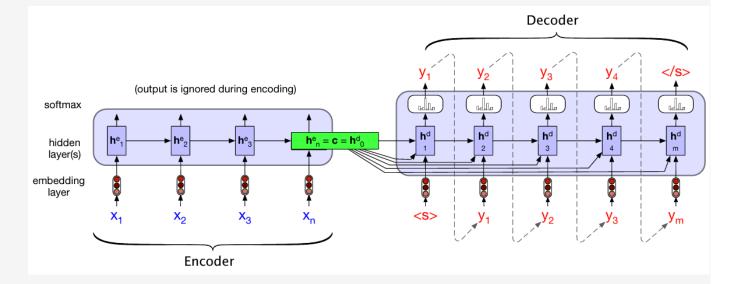
# Using RNNs for encoder and decoder

Encode the input

Pass the context at every step

$$\mathbf{h}_t^d = g(\hat{y}_{t-1}, \mathbf{h}_{t-1}^d, \mathbf{c})$$

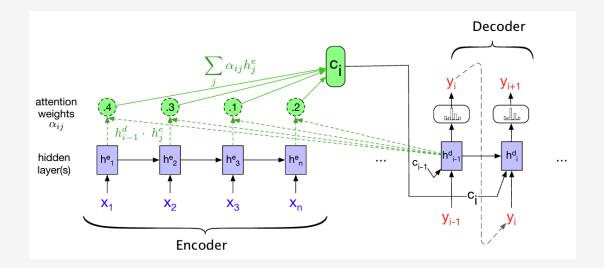
- Limitations
  - Single vector representation is a bottleneck
  - Long distance dependencies in source



# Attention – intuition

 Intuition: each token in the target should use a "personalized" context

- Access all the hidden states in the encoder
  - Still needs to have a fixed length, regardless of variable input length



The context – weighted sum of all hidden states

# Dot product attention (formally)

• Scoring function:

$$score(\mathbf{h}_{i-1}^d, \mathbf{h}_{j}^e) = \mathbf{h}_{i-1}^d \cdot \mathbf{h}_{j}^e$$

• Weight vector:

$$\alpha_{ij} = \operatorname{softmax}(\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_{j}^e))$$

$$= \frac{\exp(\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_{j}^e))}{\sum_{k} \exp(\operatorname{score}(\mathbf{h}_{i-1}^d, \mathbf{h}_{k}^e))}$$

• Personalized context:

$$\mathbf{c}_i = \sum_j lpha_{ij} \, \mathbf{h}_j^e$$

• More complex scoring functions:

$$score(\mathbf{h}_{i-1}^d, \mathbf{h}_{j}^e) = \mathbf{h}_{t-1}^d \mathbf{W}_s \mathbf{h}_{j}^e$$

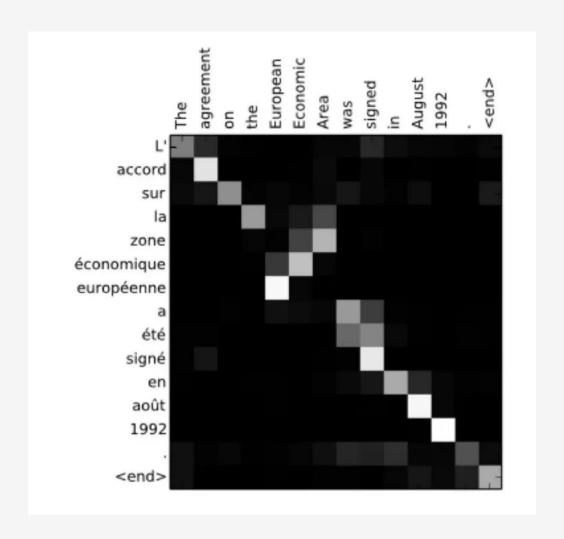
# Visualizing attention

• Linear weights are interpretable

• We can see which word is more important

Can we use attention for explainability?

How would a context of an RNN/LSTM look for enc-dec?



# Do we need LSTM?

• Original implementation: two LSTMs + attention

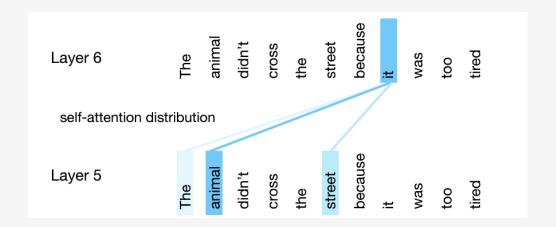
- Do we need LSTM?
  - Can process input sequentially
  - Some long-distance dependencies
  - Can't be parallelized (why?)

- Can we replace RNN/LSTM with attention?
  - "Attention is all you need"

# Self attention

- Attention is used to inform the decoder of relevant context
  - It models relations external to the model

- Self-attention can replace RNN/LSTM for compositionality
  - It models internal relations within the same layer



# The query, key, and value

- Single representation can be a bottleneck
  - The representation  $x_i$  has multiple roles
  - Dot product is commutative
  - Learning can be inefficient

• Learn different representations (projections) for each role

# The query, key, and value (2)

- We project the input vector x to three vectors that serve different purpose: "query", "key", and "value"
- Two vector operations in the original attention:
  - "Score": for indexes i and j, calculate how important is  $x_j$  for  $x_i$ : score( $x_i$ ,  $x_j$ )
  - "Scale": for index i, calculate the hidden state  $h_i$  as a weighted sum of  $x_1 \dots x_i$ :  $h_i = \sum_{j \le i} \alpha_{ij} x_j$
- Each input vector x can three different roles
  - Argument 1 in score() ["dog" in score("dog", "black")] -> query
  - Argument 2 in score() ["dog" in score("black", "dog")] -> key
  - The **value** used in scale to calculate the hidden state

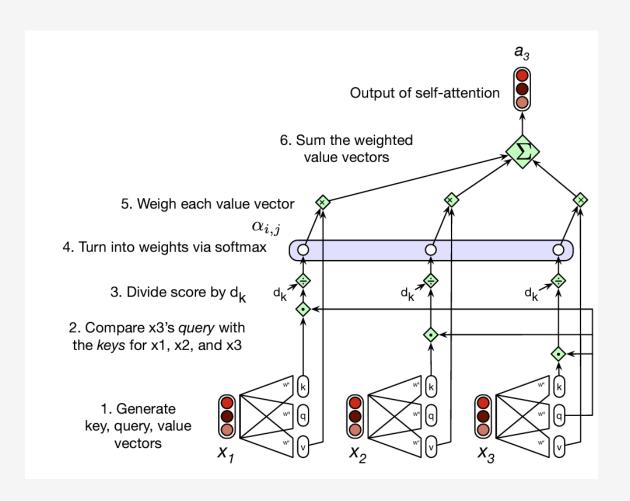
# The transformer self attention

1. 
$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^{\mathbf{Q}}; \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^{\mathbf{K}}; \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^{\mathbf{V}}$$

2. and 3. 
$$\operatorname{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}$$

$$\alpha_{ij} = \operatorname{softmax}(\operatorname{score}(\mathbf{x}_i, \mathbf{x}_j)) \ \forall j \leq i$$

5. and 6. 
$$\mathbf{a}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{v}_j$$

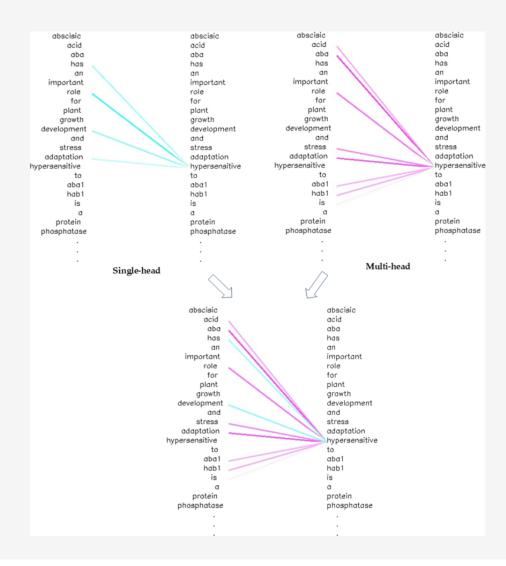


### Multiheaded self-attention

- Instead of using a single self attention, we can use multiple
  - Each "head" has its own weights W<sup>Q</sup>, W<sup>K</sup>, W<sup>V</sup>
  - The outputs of all heads are concatenated and projected to input dimensions
- Formally:

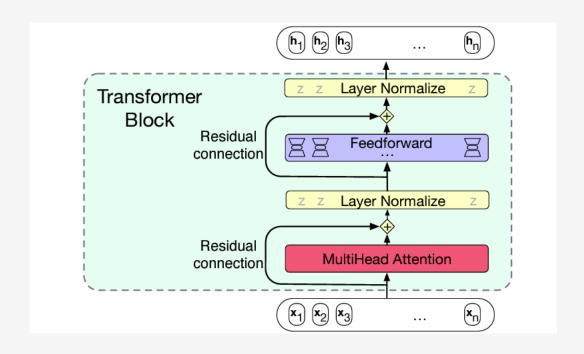
$$\mathbf{Q} = \mathbf{X} \mathbf{W}_i^Q \; ; \; \mathbf{K} = \mathbf{X} \mathbf{W}_i^K \; ; \; \mathbf{V} = \mathbf{X} \mathbf{W}_i^V \\ \mathbf{head}_i = \mathrm{SelfAttention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) \\ \mathbf{A} = \mathrm{MultiHeadAttention}(\mathbf{X}) = (\mathbf{head}_1 \oplus \mathbf{head}_2 ... \oplus \mathbf{head}_h) \mathbf{W}^O$$

- Intuition:
  - Similar to using multiple filters in CNN



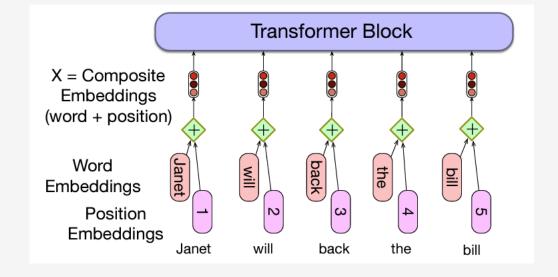
# The transformer block

- Residual connection
  - Copy the input of a layer to its output
- Layer normalize
  - Rescale each x vector to 0-mean with STD=1
- Feedforward
  - Apply the same fully connected FFN to each x



# Encoding the Input. Positional Embeddings.

- Semantic embeddings
  - One-hot encoding maps to a row in a matrix
- Positional embeddings
  - One embedding for each position
  - Learnable; Same dimension as semantic
- Add semantic and positional embeddings



Why do we need positional embeddings?

# Using functions for positional embeddings

Learning representations for positions can be a problem – data sparsity

- Using mathematical functions to encode position as a vector
  - Using the position, calculate (deterministically) a vector representation
  - OG transformer approach using sine and cosine

Same underlying concept – use positional embedding to modify the semantic embedding

# Positional embeddings with sine and cosine

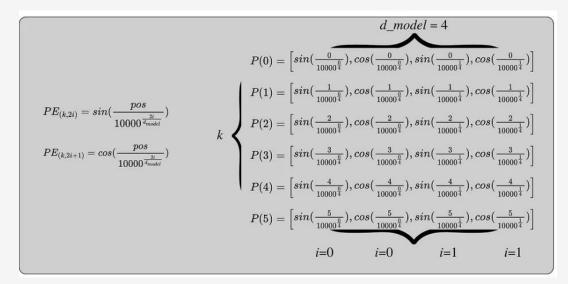
• Given: Input length L, number of dimensions d, constant n

• For each 
$$k = 0$$
 to  $L - 1$ :

• For each  $i = 0$  to  $\frac{d_{model}}{2}$ :

•  $PE_{(k,2i)} = sin(\frac{k}{\frac{2i}{model}})$ 

•  $PE_{(k,2i+1)} = cos(\frac{k}{\frac{2i}{model}})$ 



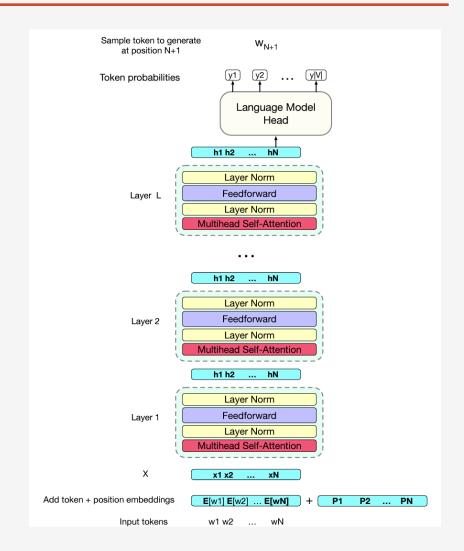
- Generate even dimensions using sin, odd dimensions using cos
  - Example with L=6, d=4, n=10000

# A final transformer representation for LM

Token + positional embedding

Multiple stacked transformer blocks

- A classification head
  - To train, we need a task and an error function
  - Language modeling with weight tying and sampling



# The original transformer

# An encoder-decoder architecture using two transformers

• The original transformer is an encoder-decoder used for machine translation

Both encoder and decoder have 6 stacked layers

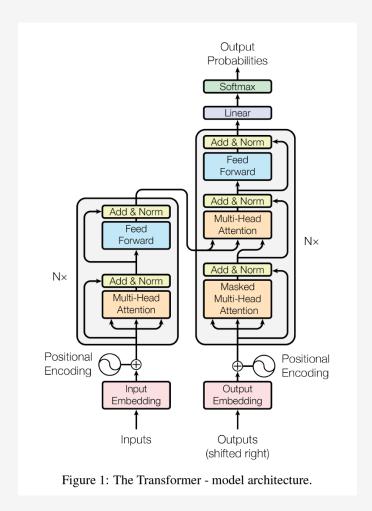
• 8 multiheads, 64 dimensions per head, hidden size of 512

Sin/Cos positional embeddings

# Image

- Encoder
  - Bi-directional attention can "see" all tokens
  - Follows the architecture we have seen last week

- Decoder
  - Causal attention
  - Additional Multiheaded Attention
    - Why do we need it?
    - What would be the Q, K, V used by it?



# Training configuration

- Training set:
  - 4.5 million En-De sentence pairs; 36 million En-FR sentence pairs
- Hardware and time:
- Parameters and specifications:
  - 65 million parameters for base; 213 million for large
  - 37k BPE token vocabulary for EN-DE; 32k for EN-FR

# Text generation from a probability distribution

• The output of a neural LM is a probability distribution

- How do we choose which word to generate?
  - Process called "decoding"
  - Efficient decoding is still a challenge
  - Any suggestions?

# Random sampling

• Random sampling – choosing a word at random, according to its probability

• Pop quiz: When do we stop?

- Objectives of sampling:
  - Quality: how good (coherent/likely/factual) is the generated text
  - Diversity: how boring/repetitive/biased is the generated text
  - Can these objectives be aligned?

# Restricting the sampling

- Greedy sampling always pick the most probable word
- Top k sampling randomly sample one of the k most probable words (re-scaling the probability to sum to 1)
  - How would greedy and top k perform in terms of quality and diversity?

- Top p sampling select tokens that represent p percentage of the probability mass
- Temperature sampling modify the probability distribution
  - Low temperature(<1) more probability to frequent tokens; High temperature more probability to unfrequent
  - How: divide the logit by temperature:  $y = softmax(u/\tau)$

# Training a transformer model

- Original transformer is trained on translation data
  - Uses bilingual data
- Calculate the error at each token (use teacher forcing)

Aggregate the error across the target language (e.g. French)

Backpropagate the error through both encoder and decoder

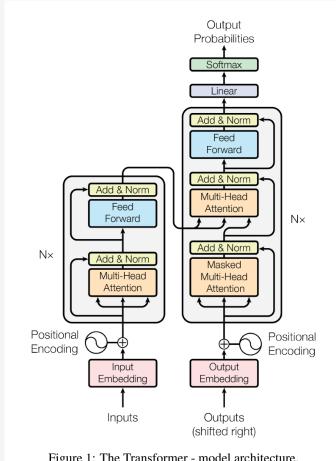


Figure 1: The Transformer - model architecture.

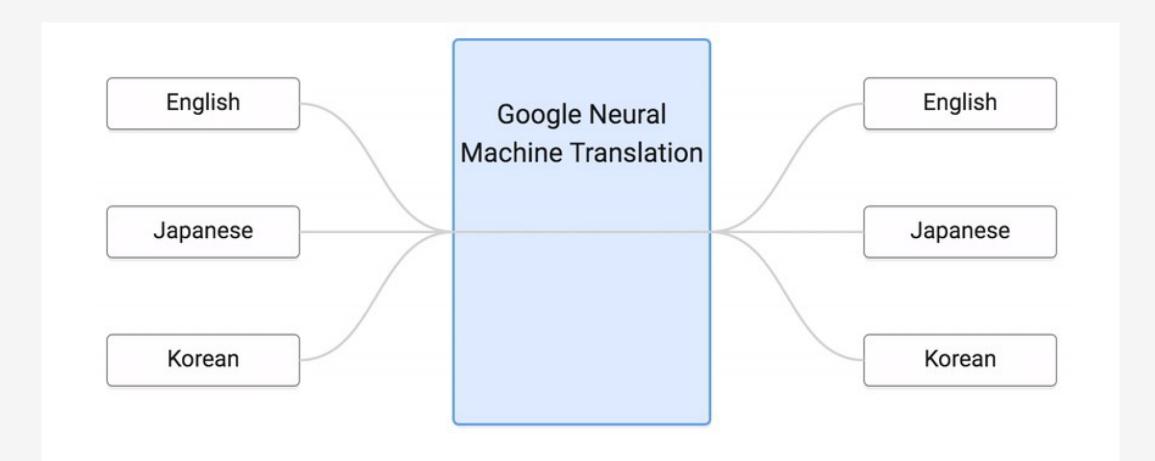
# Multilingual NMT

- To train encoder-decoder for EN-DE, you need bilingual data in EN-DE
  - E.g., books translated from EN to DE

To train encoder-decoder for EN-FR, you need bilingual data in EN-FR

Do you need bilingual data for every pair that you want to train?

# Multilingual NMT



https://research.googleblog.com/2016/11/zero-shot-translation-with-googles.html

# Transfer Learning BERT and GPT

# The concept of transfer learning in vision

Transfer learning has ben used in vision for a while

- Pretrain and finetune idea
  - Pretrain to capture general features and properties
  - Finetune to learn task-specific weights and compositions

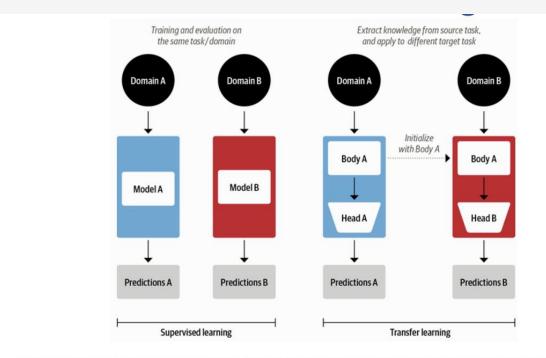
- Can we do that for language?
  - Embeddings have some limited success

# Supervised learning vs Transfer learning

 What are the goals and benefits of transfer learning?

What are some potential issues or risks?

 Are there any other paradigms that you can think of in that area?

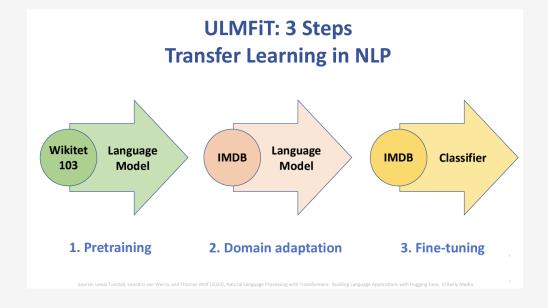


Source: Lewis Tunstall, Leandro von Werra, and Thomas Wolf (2022), Natural Language Processing with Transformers: Building Language Applications with Hugging Face, O'Reilly Media.

# ULMFiT (Howard and Ruder et al., 2018)

- "Universal Language Model Finetuning"
- Training a language model for "inductive transfer learning"
  - Model trained on a source task (language modeling)
  - Finetuned with limited data on target task

Language modeling – the analogy of ImageNet



Base model - BiLSTM

# ULMFiT Pipeline

- General-domain LM pretraining
  - Train BiLSTM on Wikipedia
- Target-task LM finetuning
  - Change the LM so it predicts words in a specific domain (e.g. IMDB)
  - Use dynamic learning rate techniques to facilitate training
- Target-task classifier finetuning
  - Add additional layers (heads) for classification: batch normalization, dropout, relu, and a final softmax

# ULMFiT Pipeline

Which parts are reused?

• What happened with last layers?

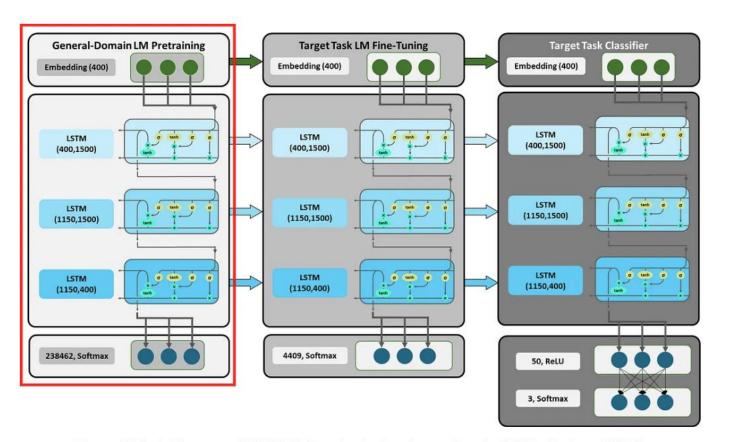


Figure 5: Block Diagram of ULMFiT in Text Analysis — Image from by <u>HU-Berlin</u> from <u>GitHub</u>

# Layer Freezing and Catastrophic Forgetting

- Catastrophic forgetting is an (unsolved) challenge in transfer learning
  - How to know what to learn and what to forget?
  - Overfitting to the task

- Freezing lower layers
  - Reducing training time
  - Reducing catastrophic forgetting and overfitting
  - Dynamic un-freezing (typically from top to bottom)

# Transfer learning and Transformers

- The original transformer was designed for encoder-decoder models
  - Initial application: Machine learning

- Soon after:
  - Encoder models: BERT, ROBERTA, DistilBERT
  - Decoder models: GPT, GPT2

• Reusing the concepts of ULMFiT, enabling transfer learning for multiple tasks

#### The decoder transformer: GPT

- GPT1 combines different concepts we know so far
  - The standard transformer block
  - Neural Language Modeling
  - Transfer learning capabilities

- Intuition:
  - Generative pre-training
  - Discriminative finetuning

# Training GPT

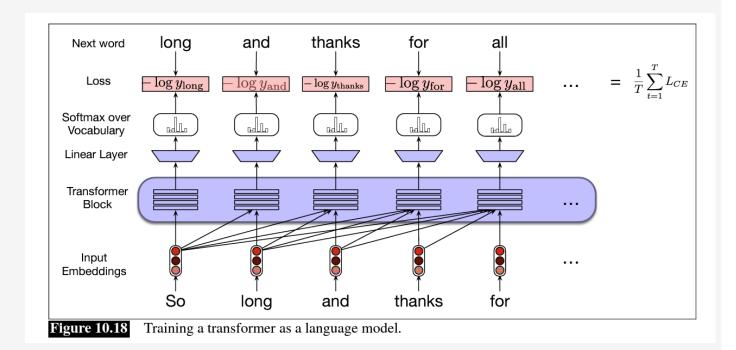
- Self-supervision
- Maximizing the likelihood of the text:

$$L_1(\mathcal{U}) = \sum_{i} \log P(u_i|u_{i-k}, \dots, u_{i-1}; \Theta)$$

Minimizing cross entropy loss

$$L_{CE}(\hat{\mathbf{y}}_t, \mathbf{y}_t) = -\log \hat{\mathbf{y}}_t[w_{t+1}]$$

• Trained on the Book Corpus (7000 books)



#### Finetuning GPT

- After pretraining, use the hidden state at last layer
- Add a last linear layer with m neurons (m = number of classes)
- Predict the target class:

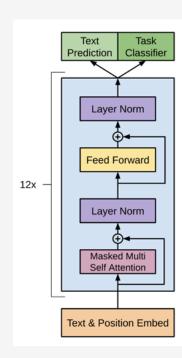
$$P(y|x^1,\ldots,x^m) = \operatorname{softmax}(h_l^m W_y).$$

Maximize the probability of the correct labels (need labeled data)

$$L_2(\mathcal{C}) = \sum_{(x,y)} \log P(y|x^1, \dots, x^m).$$

Combining both losses together

$$L_3(\mathcal{C}) = L_2(\mathcal{C}) + \lambda * L_1(\mathcal{C})$$



# Task specific input transformations

- Out-of-the-box GPT can do:
  - Text generation / Next word prediction
  - Text classification

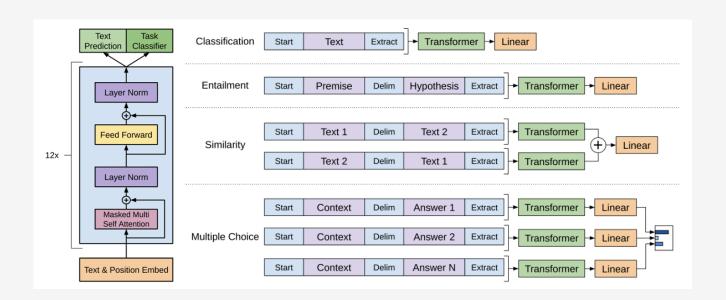
- How can it perform paraphrase identification?
  - "Is text 1 the same as text 2"
  - Suggestions?

#### Task specific input transformations

Task reformulating

Using special tokens (sep, start/end)

Comparing separate "streams"



- Task design is a non-trivial task
  - Task formulation; Data format; Metrics and Evaluation

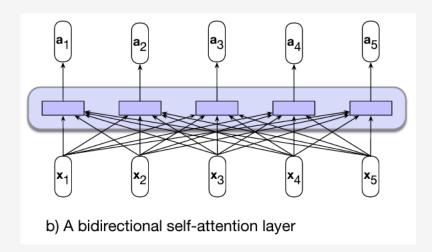
#### The encoder transformer

• The encoder in "attention is all you need"

• Same architecture as the decoder

- Bi-directional self-attention
  - All key/query values, no masking

• Better for encoding source information



#### Encoder transformer for classification

Can an encoder be better for classification?

- Follow the ULMFiT approach
  - Pretrain on a generic task
  - Add task specific layer and finetune

- How do we pretrain?
  - We cannot use "next word prediction", why?

#### The encoder transformer: BERT

- The original encoder-only transformer
- An English-only sub-word vocabulary consisting of 30,000 tokens
  - Most of the modern algorithms use subwords tokenizers and embeddings
- 768 hidden size
- 12 layers, 12 heads in each multi-head attention
- 100M parameters
- Trained on two tasks: Masked Language Modeling and Next Sentence Prediction

# Masked language modeling objective

- Based on "cloze" tasks:
  - "Can I have a \_\_\_\_ of water, please?"
  - · Does that remind you of something?
- Masked Language Modeling (MLM)
  - Randomly sample tokens from the text and perform alternations
  - Predict the original inputs for each position

# MLM and masking

- Rate of sampling 15% of the input
- Alternations on sampled tokens
  - replace them with [MASK] (80%)
  - replace them with another word (10%)
  - do nothing (10%)
- Use the attention mechanism to calculate the hidden state at all masked positions
  - Calculate cross entropy loss and backpropagate

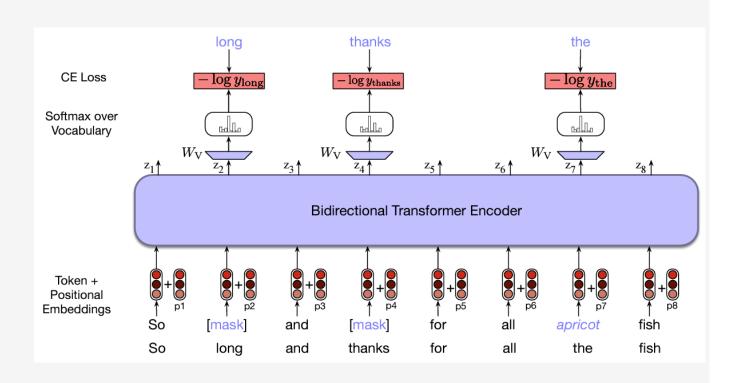
#### MLM (visualization)

In Traditional LMs we predict next token

• In MLM we predict "current" token

All words participate in attention

Only "masked" tokens participate in learning



# MLM Efficiency and pop quizes

• Is MLM a self supervised approach?

How efficient is MLM compared to traditional LM

- Why didn't we have MLM in original encoder-decoder?
  - How did we train the encoder there?

#### Next Sentence Prediction

• MLM predicts relationships between words

• Transformers want to also process sentences

- Next sentence prediction task
  - Given two sentences, predict whether they are a pair of adjacent sentences

#### Next sentence prediction. The CLS token.

- Next sentence prediction
  - 50 % true adjacent pairs
  - A special [CLS] token added at the beginning
  - A special [SEP] token added between texts
  - Special "sentence position" (first/second) are added to input

When predicting the sentence relation, we use the CLS as an input to softmax

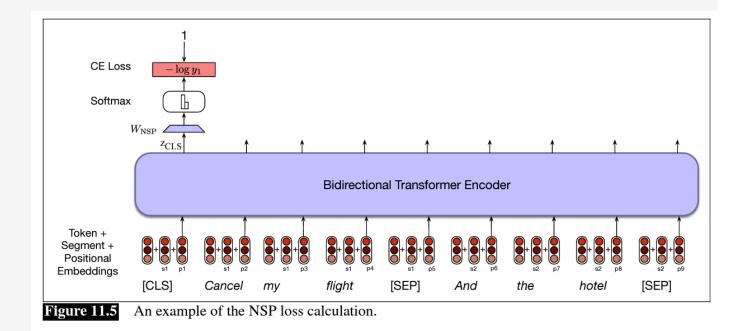
#### The CLS token

 Sentence predictions by BERT are based on the CSL token

$$y_i = \operatorname{softmax}(\mathbf{W}_{\mathbf{NSP}} h_i)$$

Why do we want to use the CLS token?

 Is there any other way to predict the sentence relation?



# Representing sentences

• A recurring problem

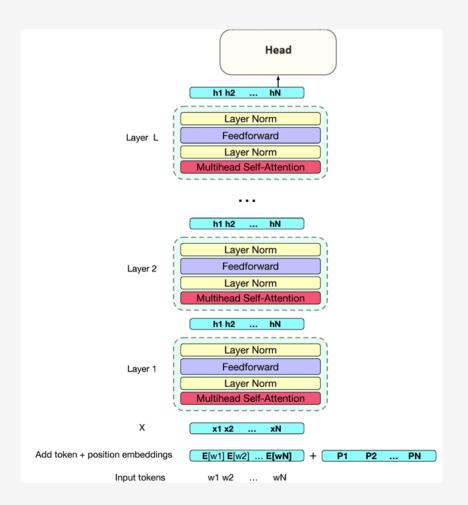
- Word representations
  - Static or contextual

- How do we represent sentences or documents?
  - What strategies have we used before?

#### Representing sentences

- What strategies can we use to encode the full text?
  - Vector addition
  - Vector concatenation
  - Let the head deal with it
  - Which vector representations are we to use?

- BERT uses the CLS token instead
  - Learning compositionality as a "special token"



# Training BERT

Combination of Wikipedia and Book Corpus

Pairing of sentences (true/false pairs)

• Masking of tokens within both sentences

Combining the MLM loss and NSP loss

• Which other architecture had two losses? What were they?

# Finetuning BERT

The same conceptual idea as in ULMFiT and GPT

• Train BERT on web data

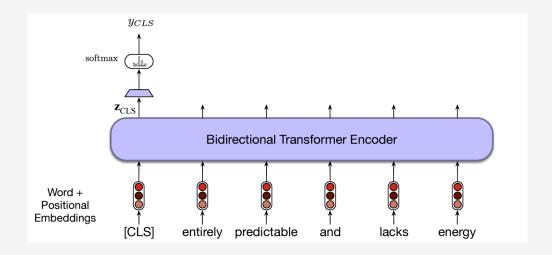
- Change the classifier "head" and finetune
  - What would we use as an input to the classifier head?

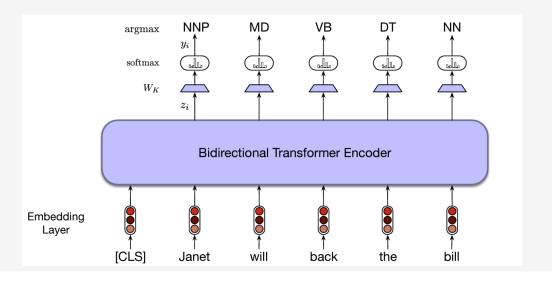
What weights are we updating during finetuning?

#### Adapting other tasks to work with BERT

- How would we perform paraphrase identification?
  - What is the input/output/classification process?

- Performing other tasks:
  - Extractive QA
  - Sequence labeling





## Popularity and use of encoder-only models

- Original BERT model achieved SOTA on almost all benchmarks
- Improved models:
  - ROBERTA, DistilBERT, ELECTRA, ALBERT

Reframing multiple tasks as text classification

- Much better than GPT and GPT2
  - The arrival of GPT3 and increasing scale of training resulted in paradigm shift

## What information do transformers capture?

• Pipeline approaches follow a (linguistic) logic

• End-to-end neural models are optimized for a task

• Difficult to interpret

• Pretraining for CV follows "meaningful" patterns

What patterns do linguistic pretraining follow?

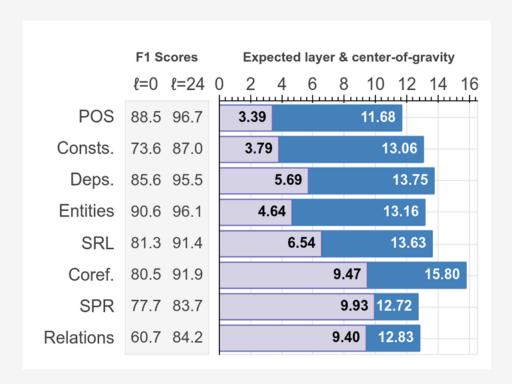
#### Bert rediscovers the classical NLP pipeline

- Probing different layers of BERT for linguistic information
  - Lower layers capture local information; Higher layers capture complex structures
  - Sometimes information can be spread across multiple layers
- Tenney et al. (2019)
  - Does BERT encode traditional NLP preprocessing steps: POS tagging, syntactic parsing...
  - Does BERT follow the same order of operations?
  - What happens with a sentence as it goes through BERT?

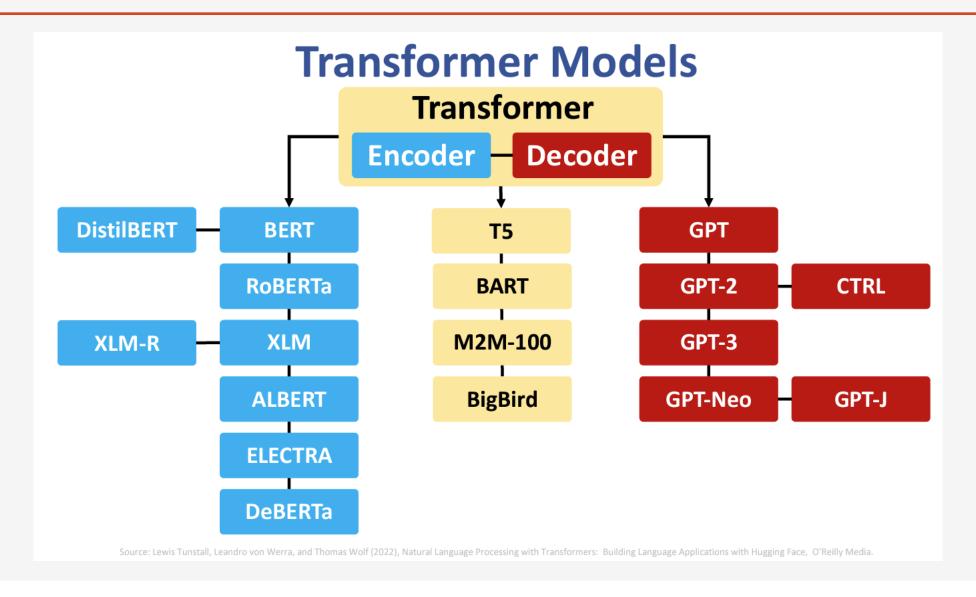
#### Bert rediscovers the classical NLP pipeline (2)

- Two different evaluation criteria
  - Purple at which layer is most of the information encoded
  - Blue average layer "used"

- Different linguistic properties are "discovered" in order
  - "Early" properties have a long "tail"



#### The transformer family tree



# Scaling laws

• V	Vhat makes	LLMs	better	and	how	much	better	can	they	be?
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- The performance of LLMs depends on three factors:
  - Model size
  - Data size
  - Compute power
- The (expected) performance of different models can be represented as a function of those factors
  - Kaplan et al. (2020) proposes "scaling laws" for LLMs

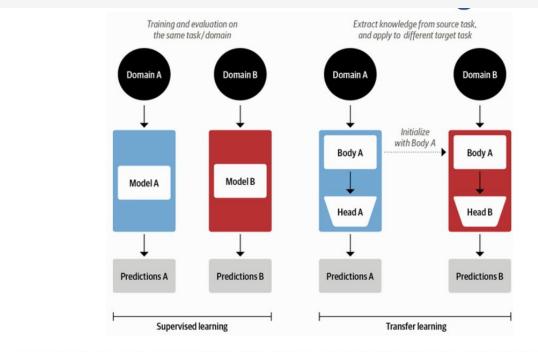
# Path towards AGI? Zero-shot and Few-shot learning

## Supervised Learning vs Transfer Learning

• In supervised learning, we train from scratch

• In transfer learning, we only change the head

- Can we go further in reducing need for data?
  - How do humans perform tasks?



Source: Lewis Tunstall, Leandro von Werra, and Thomas Wolf (2022), Natural Language Processing with Transformers: Building Language Applications with Hugging Face, O'Reilly Media.

## NLP Paradigm shifts

- Several key papers driving paradigm shifts in NLP
  - Word2Vec Mikolov et al. (2013)
  - End-to-end LSTM/BiLSTM and GRU multiple papers in 2014
  - Attention Bhadanau et al. (2014)
  - Transformer Vaswani et al. (2017)
  - BERT Devlin et al. (2019)
  - GPT 3 Brown et al. (2020)
  - Instruct-GPT Ouyang et al. (2022)

#### GPT3

- A major shift in NLP paradigm
  - Arguably the largest shift since moving from pipeline to end-to-end models

- Introduced few-shot and zero-shot learning
  - Teaching a model to perform a task without changing the weights (!)

In-context learning and prompt engineering

#### GPT3 and current LLMs

Almost all of current chat-enabled LLMs are based off the concepts in GPT3

- Newer models are performing better
  - More parameters; larger and better datasets
  - Additional training: supervised and RLHF finetuning
  - Human-driven and machine-driven prompt engineering

- GPT3 can, in principle, do anything that modern LLMs can
  - The difference is in the implementation, not in the core concepts (!)

#### Few-shot and Zero-shot learning

- The problem
  - Getting training data is complex and expensive (there are far more tasks than datasets)
  - Overfitting (to spurious correlations)
  - Humans don't need large training data for all tasks
- The goal
  - One model that can perform multiple tasks
  - In-context learning
  - AGI?

# In-context learning vs supervised/transfer learning

- Using the input to specify the task
- Consider the following inputs to a transformer model:
  - "I like this movie, it's the best in the Avengers series!"
  - "I bike to work every day. <SEP> I drive to work every day."
- What is the task? What is the output?
  - The task is what you train the model to do
  - The first sentence can be an input to a NER model
  - The second sentence can be an NLI task or a similarity task

#### In context learning

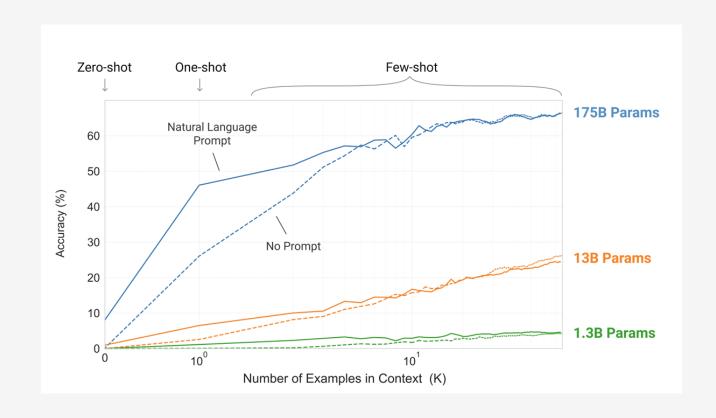
- Now consider the following inputs:
  - "What is the sentiment of the following text: I like this movie, it's the best in the Avengers series!"
  - "Do those sentences contradict each other: I bike to work every day. <SEP> I drive to work every day."

- How do we achieve in-context learning?
  - GPT3 paper argues that scale and emerging properties are the answer
  - Increasing model size from 17B to 175B

# In-context learning and model size

- Two key factors
  - Model size
  - Number of examples

Model size -> "emerging properties"



#### Zero- One- and Few-shot learning

Three different experimental conditions

No gradient update or finetuning

• The only difference – number of examples

The three settings we explore for in-context learning

#### Zero-shot

The model predicts the answer given only a natural language description of the task. No gradient updates are performed.

```
Translate English to French: ← task description

cheese => ← prompt
```

#### One-shot

In addition to the task description, the model sees a single example of the task. No gradient updates are performed.

```
Translate English to French: ← task description

sea otter => loutre de mer ← example

cheese => ← prompt
```

#### Few-shot

In addition to the task description, the model sees a few examples of the task. No gradient updates are performed.

```
Translate English to French: task description

sea otter => loutre de mer examples

peppermint => menthe poivrée

plush girafe => girafe peluche

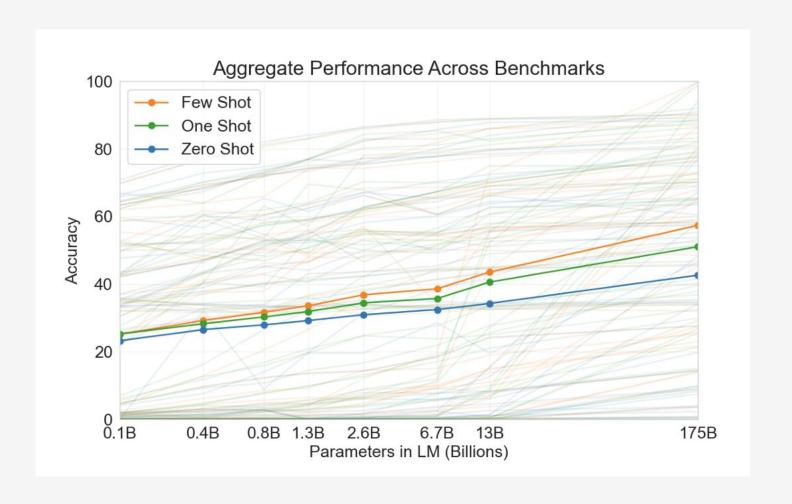
cheese => prompt
```

# In-context learning and model size

Same model

Different sizes

Different number of examples



#### Mode architecture

- Same as GPT2, scaled to 175B params
  - 96 layers
  - 96 attention heads
  - 128 d per head -> 12k d for the hidden state

- Causal attention, trained on LM task
  - Trained on Common Crawl (1 trillion words) + data filtering
  - Additional curated high-quality datasets

#### Compute used for training



#### GPT and contemporary LLMs (2)

GPT3 paved the path towards contemporary LLMs

- Modern LLMs build upon GPT3 focusing on several key directions
  - Improved training practices (instruction tuning)
  - Increased model size
  - Increased data size and data quality
  - Multimodality
  - Prompt engineering