Pretraining and Finetuning

He He

NEW YORK UNIVERSITY

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Last week

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- **Decoders**: vectors to tokens
- **Key difference**: (autoregressive) decoders cannot look at the future
  - Need causal masking
  - Sequential output

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- Can you use a decoder to encode text?

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Representation learning

Recap: What are good representations?

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Examples: negative the food is good but doesn't worth an hour wait

- Simple features (e.g. unigram BoW) require complex models.
- Good features only need simple models (e.g. linear classifier) .

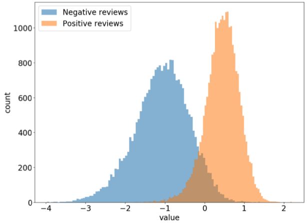

Figure: Sentiment neuron [Radford et al., 2017]

Representation learning

What can we do with good representations:

- Learning with small data: fine-tuning learned representations
- Transfer learning: one model/representation for many tasks
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- Metric learning: get a similarity metric

How to obtain such a representation:

- Training a neural network on any task gives us a representation good for *that task*.
- But on which task can we learn good *general* representations?

What can we learn from word prediction given context?

- The cats that are raised by my sister ________ sleeping.

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- The cats that are raised by my sister ________ sleeping. *syntax*
- Jane is happy that John invited ________ friends to his birthday party.

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- The boy is ________ because he lost his keys. *commonsense*
- John took 100 bucks to Vegas. He won 50 and then lost 100. Now he only has ________ to go home.

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Text contains a surprisingly large number of tasks!

Self-supervised learning for representation learning

Key idea: predict parts of the input from the rest

- No additional supervision is needed—both input and output are from the raw text data.
- Easy to scale—massive amount of text on the Internet.
- Learned representation is general—useful for any tasks that can be performed in textual mode.

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How is this different from skip-gram / CBOW?

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Approach:

- **Pretrain**: train a model using self-supervised learning objectives on large data.
- **Finetune**: update part or all of the parameters of the pretrained model on labeled data of a downstream task.

A bit of history

- Pretrain an RNN model on unlabeled data and finetune on supervised tasks [Dai et al., 2015] [ULMFiT; Howard et al., 2018]
  - Promising results on a small scale

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  - First impactful result in NLP
- Pretrain a Transformer model and finetune on supervised tasks
  - GPT [Radford et al., 2018], BERT [Devlin et al., 2018]
- Scale pretrained transformer to larger data and compute
  - Can directly answer user questions and solve many tasks, e.g., ChatGPT, Claude, Deepseek-chat

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Challenges in tokenization

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- A long tail of rare words
  Neologism, terminologies, misspelling, informal text, etc.
- A mixture of multiple natural languages, programming languages, special symbols
  Low-resource language, math equations, code-switching, emoji, etc.
- Efficiency
  Trade-off between vocab size and sequence length, latency

Subword tokenization

The most widely adopted solution: decomposing words into subword units

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  `bioorthogonal` $\rightarrow$ `bio ##ortho ##gonal`

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  `Donaudampfschifffahrtsgesellschaft` → `Donaudampf ##schiff ##fahrts ##gesellschaft` (German compound noun meaning "Danube steamship company")
- Efficiency
  Balancing granularity and efficiency: reducing token count without losing meaning

Byte pair encoding (BPE)

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BPE:

- Origin: a compression algorithm that iteratively replace the most common character sequences by a single symbol, e.g., $\texttt{un} \rightarrow \texttt{A}$
- Start with individual characters as tokens
- Merge the most frequent pair of tokens and treat them as a single token
- Update the input with the new token and repeat the process
- Output: tokenized text and a set of merge rules

BPE Example (Step-by-Step)

Initial Sequence:

- Words: `banana`, `band`, `ban`
- Initial tokenization (by character):
  - `b a n a n a`
  - `b a n d`
  - `b a n`

BPE Example (Step-by-Step)

Initial Sequence:

- Words: `banana`, `band`, `ban`
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Step 1: Count Pairs

- What is the most frequent pair:

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Step 1: Count Pairs

- What is the most frequent pair: `a n`

Step 2: Merge

- New merge rule: `a`, `n` $\rightarrow$ `an`
- Updated tokenization:
  - `b a n a n a` $\rightarrow$
  - `b a n d` $\rightarrow$
  - `b a n` $\rightarrow$

BPE Example (Step-by-Step)

Step 3: Count Pairs Again

- Updated tokenization:
  - `b an an a`
  - `b an d`
  - `b an`
- Most frequent pair: `b an`

Step 4: Merge

- New merge rule: `b, an` $\rightarrow$ `ban`
- Updated tokenization:
  - `ban an a`
  - `ban d`
  - `ban`

BPE: practicalities

- Repeat the process until the desired number of merges or vocabulary size is reached (a hyperparameter to decide). Typically vocabulary sizes are 32-64K.
- Break ties deterministically, e.g., lexicographical order, occurrence in the corpus etc.
- Use bytes as the initial tokens (adopted by GPT-2)
- Variants: instead of merging the pair with the largest frequency, **WordPiece** merges the pair that maximizes the log likelihood of the training data, i.e. Merge `a, b` if

$$\log p(a, b) - \log p(a)p(b)$$

  is the largest among all pairs

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Current pretrained models are all transformer based.

Encoder models

An encoder takes a sequence of tokens and output their *contextualized* representations:

$$h_1, \ldots, h_n = \mathrm{Encoder}(x_1, \ldots, x_n)$$

We can then use $h_1, \ldots, h_n$ for other tasks.

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How do we train an $\mathrm{Encoder}$?

- Use any supervised task: $y = f(h_1, \ldots, h_n)$
- Use self-supervised learning: predict a word from its context

Masked language modeling

? language processing is ?

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Learning objective (MLE):

$$\max \sum_{x \in \mathcal{D}, i \sim p_{\text{mask}}} \log p(x_i \mid x_{-i}; \theta)$$

- x: a sequence of tokens sampled from a corpus $\mathcal{D}$
  natural language processing is fun
- p_{mask}: mask generator
  Sample two positions uniformly at random, e.g., 1 and 5
- x_{-i}: noisy version fo x where x_i is corrupted
  [MASK] language processing is [MASK]

BERT: objective

- **Masked language modeling**:
  - Randomly sample 15% tokens as prediction targets
  - Replace the target tokens by `[MASK]` or a random token, or leave it unchanged

    cats are cute $\rightarrow$ cats `[MASK]`/is/are cute
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    cats are cute $\rightarrow$ cats `[MASK]`/is/are cute
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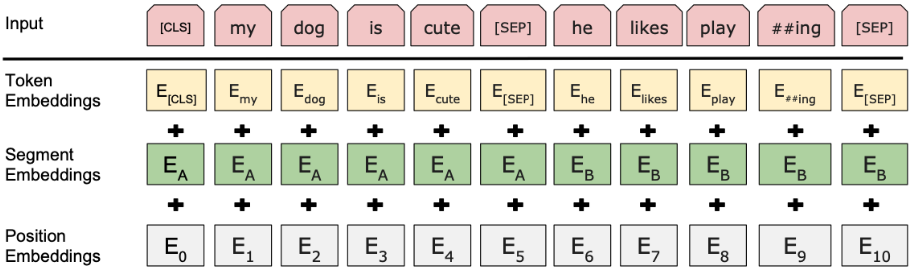
- **Next sentence prediction**: predict whether a pair of sentences are consecutive

$$\max \sum_{x \sim \mathcal{D}, x_n \sim p_{\text{next}}} \log p(y \mid x, x_n; \theta)$$

  - x_n: either the sentence following x or a randomly sampled sentence
  - y: binary label of whether x_n follows x
  - Later work has shown that this objective is not necessary

BERT: architecture



- Tokenization: wordpiece (similar to byte pair encoding) (see details)

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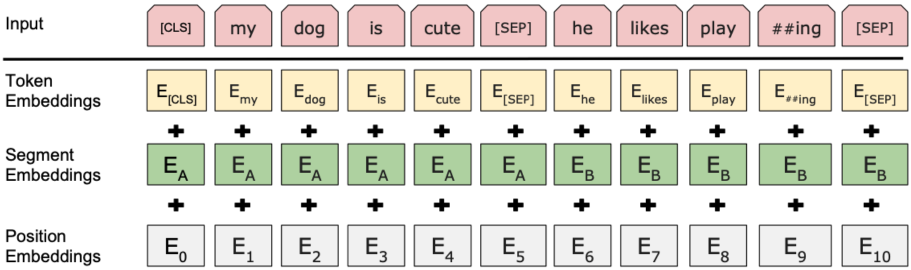

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- `[CLS]`: first token of all sequences; used for next sentence prediction

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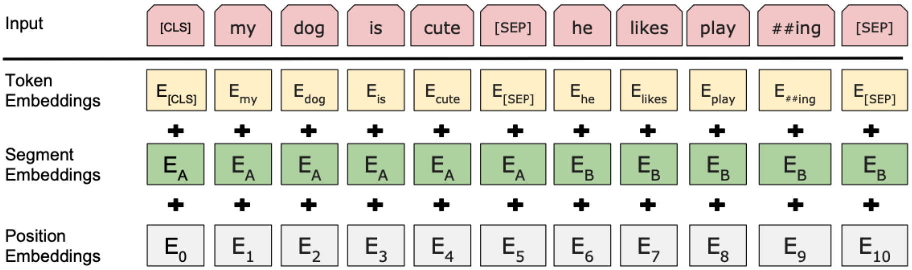

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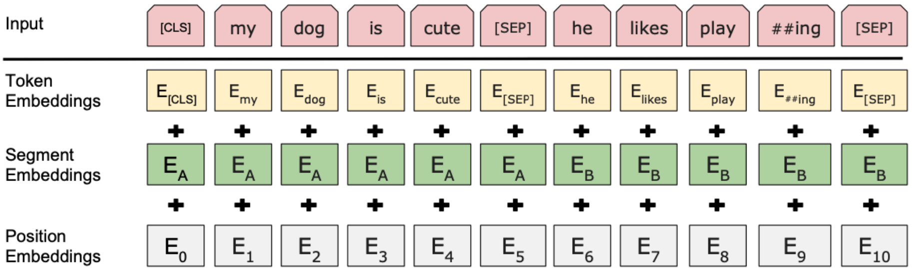

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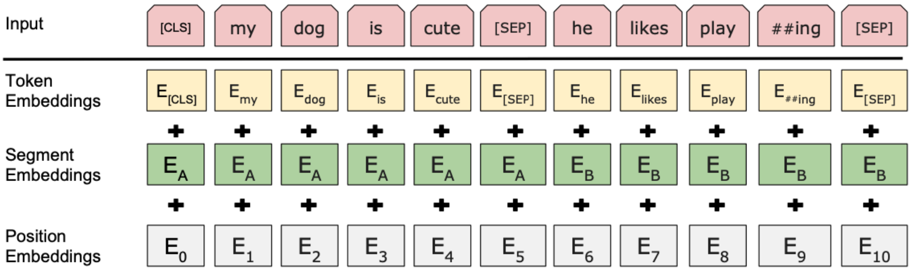

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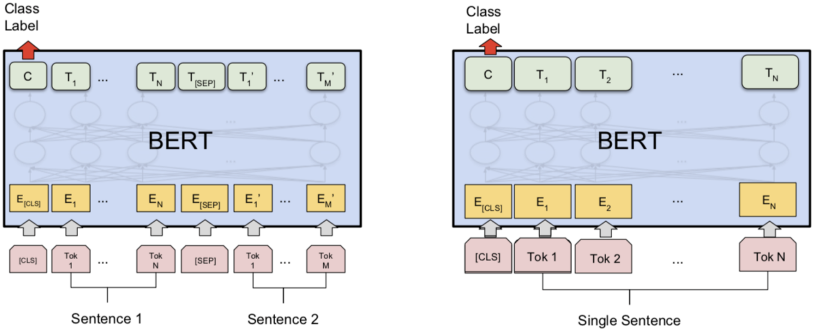
- `[CLS]`: first token of all sequences; used for next sentence prediction
- Distinguish two sentences in a pair: `[SEP]` and segment embedding
- Learned position embedding
- 12 (base; 110M params) or 24 (large; 340M params) layer Transformer

Finetuning BERT

Classification tasks: Add a linear layer (randomly initialized) on top of the `[CLS]` embedding

$$p(y \mid x) = \mathrm{softmax}(Wh_{[\mathrm{CLS}]} + b)$$



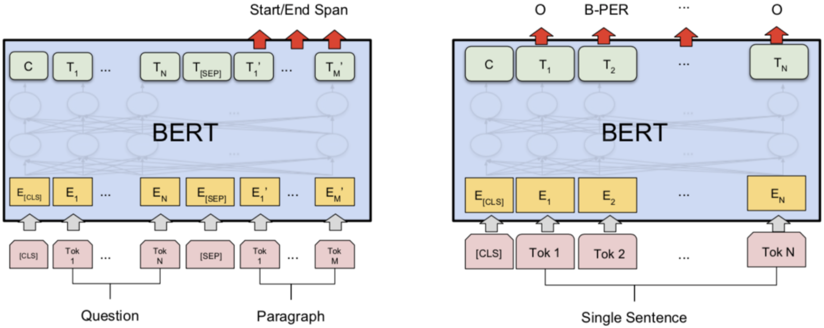
(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG

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

Finetuning BERT

Sequence labeling tasks: Add linear layers (randomly initialized) on top of every token

$$p(y_i \mid x) = \mathrm{softmax}(Wh_i + b)$$



(c) Question Answering Tasks: SQuAD v1.1

(d) Single Sentence Tagging Tasks: CoNLL-2003 NER

Finetuning BERT

- Finetune all parameters (both the newly added layer and the pretrained weights)
- Use a small learning rate (e.g., 1e-5)
- Train for a small number of epochs (e.g, 3 epochs)
- Led to SOTA results on many NLU tasks

How to generate text from BERT?

Encoder-decoder models

An encoder-decoder model encodes input text to a sequence of contextualized representations, and decodes a sequence of tokens autoregressively.

$$
\begin{aligned}
h_1, \ldots, h_n &= \mathrm{Encoder}(x_1, \ldots, x_n) \\
s_1, \ldots, s_m &= \mathrm{Decoder}(y_0, \ldots, y_{m-1}, h_1, \ldots, h_n) \\
p(y_i \mid x, y_{<i}) &= \mathrm{softmax}(W s_i + b)
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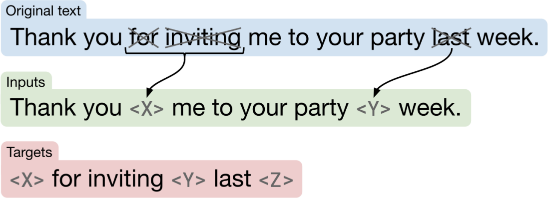
\end{aligned}
$$

How do we train the encoder-decoder?

- Use any supervised task, e.g., machine translation
- Use self-supervised learning: predict text spans from their context

Masked language modeling using an encoder-decoder

Input: text with corrupted spans
Output: recovered spans

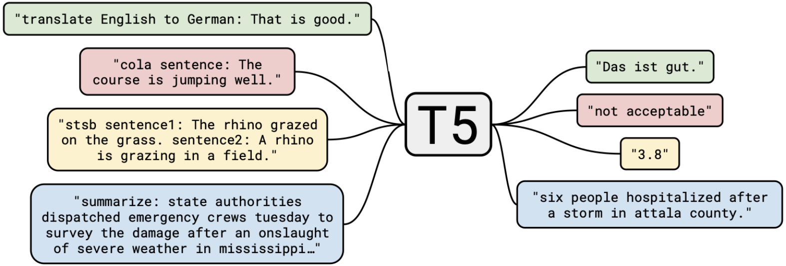


Compare with encoder-only models:

- Encoder: predict single tokens based on encoder representation
- Encoder-decoder: predict a sequence of tokens (flexibility in objective design)

T5: objective

- First train on unlabele data by **masked language modeling**
  - Predict corrupted spans as a sequence
- Then continue training by **supervised multitask learning**
  - Formulate tasks as text-to-text format using a prefix to denote the task
  - Mixing examples from different datasets when constructing batches



- Jointly training with the two objectives works slightly worse

T5: finetune

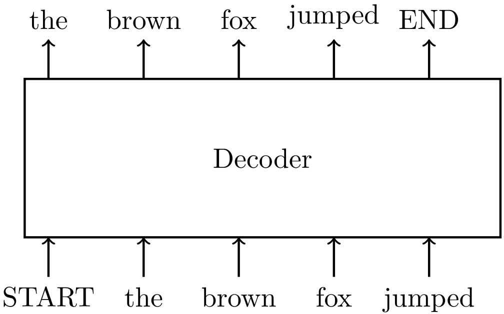
- Formulate the task in text-to-text format
- Fine-tune all parameters (similar to BERT fine-tuning)
- Advantages over encoder models: unified modeling of many different tasks including text generation

Decoder-only models

A decoder-only model predicts the next token given the prefix autoregressively.

$$s_1, \ldots, s_m = \mathrm{Decoder}(y_0, \ldots, y_{m-1}, h_1, \ldots, h_n)$$
$$p(y_i \mid y_{<i}) = \mathrm{softmax}(W s_i + b)$$

(A prefix of y can be the input.)



(more on language models later)

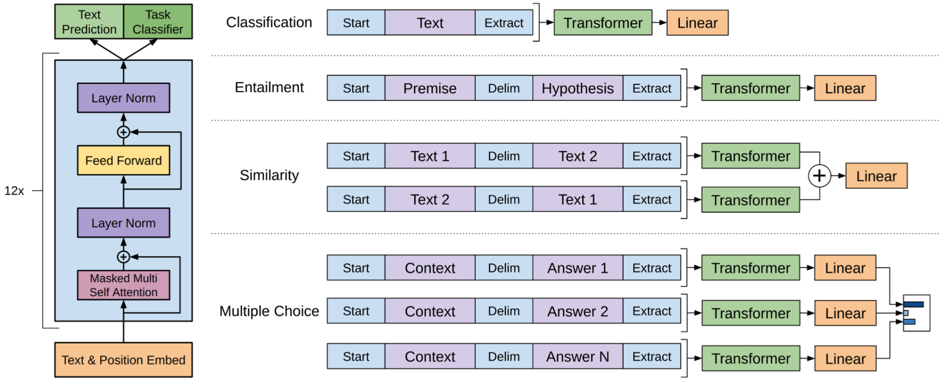
Generative Pretraining (GPT)

- **Model**: 12 layer decoder-only transformer
- **Objective**: next word prediction

$$\max \sum_{y \in \mathcal{D}} \sum_{i} \log p(y_i \mid y_{<i})$$

- **Finetuning**: auxiliary LM objective $L_{\text{task}} + \lambda L_{\text{LM}}$ (next word prediction on labeled task data)

Generative Pretraining (GPT): task-specific finetuning



- Single input: linear on top of `extract`
- Multiple input: process each input separately then aggregate

Ablation studies of GPT

Architecture, pretraining, finetuning: which is critical?

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

- Auxiliary objective only helps on larger datasets (MNLI, QQP)
- Pretrained transformer $>$ pretrained LSTM (single layer) $>$ non-pretrained transformer

Compare with BERT

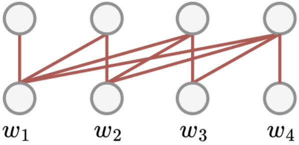
System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
$\text{BERT}_{\text{BASE}}$	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
$\text{BERT}_{\text{LARGE}}$	**86.7/85.9**	**72.1**	**92.7**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**82.1**

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

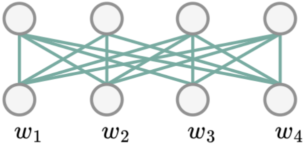
Medium-sized encoder models tend to work better than decoder-only models when finetuned

Encoder-only vs decoder-only models: attention

Decoder-only

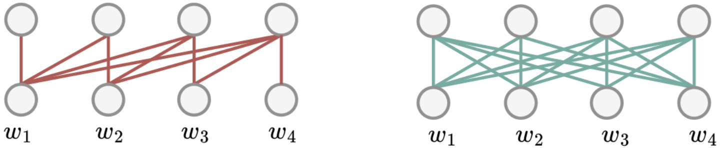


Encoder-only



Encoder-only vs decoder-only models: attention

Decoder-only Encoder-only



Encoder-only models provides better embeddings due to bidirectional attention.

Encoder-only vs decoder-only models: generation

Decoder-only models can make predictions through generation *without finetuning*

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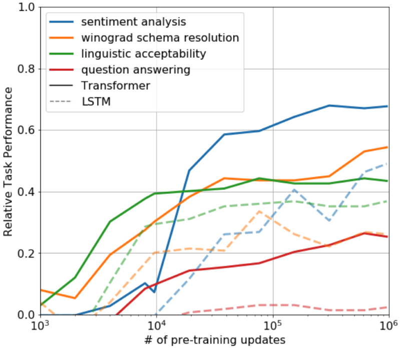

Heuristics for zero-shot prediction:

- Sentiment classification: [example] + very + {positive, negative}   *prompting*
- Linguistic acceptability: thresholding on log probabilities
- Multiple choice: predicting the answer with the highest log probabilities

Scaling trend: zero-shot performance increases during pretraining

Encoder-only vs decoder-only models: training efficiency

On each sequence:

- Encoder-only models are trained on 15% (mask rate) of the tokens
- Decoder-only models are trained on all tokens

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What about encoder-decoder models?

- Flexibility on encoder design, e.g., full attention on input context
- Limited advantage on long-form generation tasks over decoder-only model
- More resource available for decoder-only models

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Optimization for pretraining

What are challenges of optimization in pretraining?

- Numerical stability (no NaN and diverging losses)
  initialization, normalization, learning rate schedule
- Memory efficiency (work with billions of parameters)
  mixed precision, gradient accumulation

Adam optimizer

Key ideas:

- Momentum
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- Momentum
  - Motivation: having an inertia of moving in the same direction $\rightarrow$ reduce oscillation
  - How: maintain a ”memory” (moving average) of past updates
- Adaptive step size for each parameter
  - Intuition:
    flat regions (gradient changing slowly) $\rightarrow$ take larger steps
    steep regions (gradient changing fast) $\rightarrow$ take smaller steps
  - Handle sparse features well (e.g., rare words embeddings aren’t updated often)

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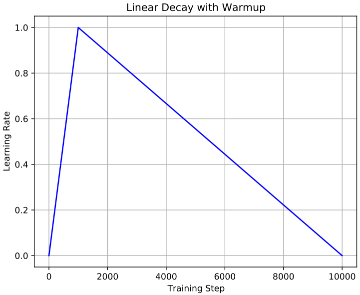
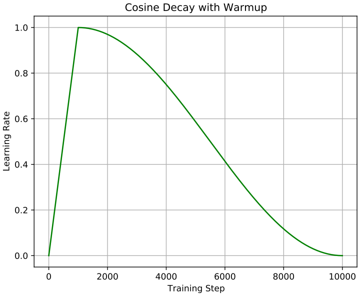
What is the memory cost of SGD vs Adam?

Learning rate schedule

- **Warmup**: don't want to start with large learning rate for stability
- **Decay**: reducing learning rate as model converges
  linear (used by BERT), cosine, exponential





Gradient accumulation

Simulate large batch training with limited GPU memory

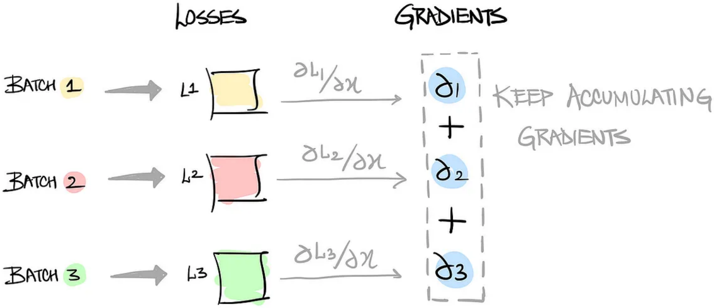


Figure: From Harshit Sharma