Pretraining and Finetuning

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October 9, 2023

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Representation learning

Architectures of pretrained models

Efficient pretraining

What are good representations?

- Enable a notion of distance over text (word embeddings)
- Contains good features for downstream tasks

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

- Simple features (e.g. BoW) require complex models.
- Good features only need sir ¹⁰⁰/₁₀₀/₁₀₀/₁₀₀¹⁰/₁₀₀¹

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

What can we do with good representations:

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

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

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?

• The cats that are raised by my sister ______ sleeping.

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

syntax

- The cats that are raised by my sister ______ sleeping. syntax
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- _____ is the capital of Tanzania.

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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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Word guessing entails many tasks related to language understanding!

Self-supervised learning

Key idea: predict parts of the input from the rest

- No supervision is needed—both input and output are from the raw data.
- Easy to scale—only need unlabeled data.
- Learned representation is general—useful for many tasks.

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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 (which provides an initialization) on labeled data of a downstream task.

- 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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- Pretrain a Transformer model and finetune on supervised tasks
 - GPT [Radford et al., 2018], BERT [Devlin et al., 2018]
- Scale the pretrained model to larger sizes
 - GPT-2 (1.5B), T5 (11B), GPT-3 (175B), PaLM (540B)
 - We will talk about 100B+ models in the third module

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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:

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

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

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How do we train an 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 ?

Masked language modeling

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Learning objective (MLE):

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

- *x*: a sequence of tokens sampled from a corpus *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

• Later work has shown that just use [MASK] is sufficient

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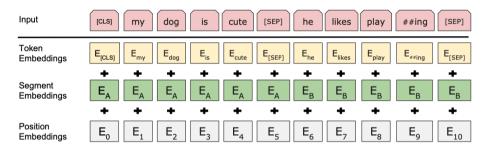
- Later work has shown that just use [MASK] is sufficient
- Next sentence prediction: predict whether a pair of sentences are consecutive

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

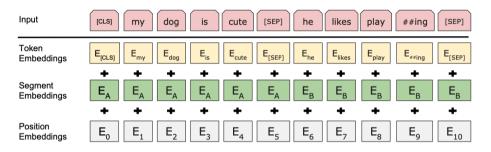
- x_n : either the sentence following x or a randomly sampled sentence
- *y*: binary label of whether x_n follows *x*
- Later work has shown that this objective is not necessary

| Input | [CLS] my dog is cute [SEP] he likes play ##ing [SEP] |
|------------------------|--|
| Token Embeddings | $\label{eq:cls} \left[\begin{array}{c} E_{my} \end{array} \right] \left[\begin{array}{c} E_{dog} \end{array} \right] \left[\begin{array}{c} E_{is} \end{array} \right] \left[\begin{array}{c} E_{cute} \end{array} \right] \left[\begin{array}{c} E_{lee} \end{array} \right] \left[\begin{array}{c} E_{he} \end{array} \right] \left[\begin{array}{c} E_{play} \end{array} \right] \left[\begin{array}{c} E_{s*ing} \end{array} \right] \left[\begin{array}{c} E_{ISEP} \end{array} \right] \left[\begin{array}{c} E_{nikes} \end{array} \right] \left[\begin{array}{c} E_{play} \end{array} \right] \left[\begin{array}{c} E_{s*ing} \end{array} \right] \left[\begin{array}{c} E_{ISEP} \end{array} \right] \left[\begin{array}{c} E_{nikes} \end{array} \right] \left[\begin{array}{c} E_{play} \end{array} \right] \left[\begin{array}{c} E_{s*ing} \end{array} \right] \left[\begin{array}{c} E_{ISEP} \end{array} \right] \left[\begin{array}{c} E_{nikes} \end{array} \right] \left[\begin{array}{c} E_{ning} \end{array} \right] \left[\begin{array}[\\ E_{ning} \end{array} \right] \left[\begin{array}[\\ E_{ning} \end{array} \right] \left[\begin{array}[\\ E_{ning} \end{array} \right] \left[\left[\\ E_{ning} \end{array} \right] \left[\left[\\ E_{ning} \end{array} \right] \left[\left[\left[E_{ning} \end{array} \right] \left[\left[\left[E_{ning} \end{array} \right] \right] \left[\left[\left[E_{ning} \end{array} \right] \left[\left[$ |
| Segment Embeddings | $\begin{array}{c} \bullet \\ \bullet $ |
| Position Embeddings | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |

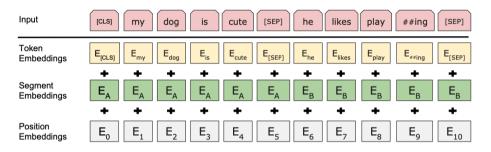
• Tokenization: wordpiece (similar to byte pair encoding) (see details)



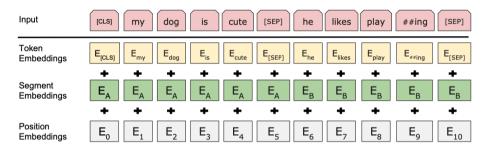
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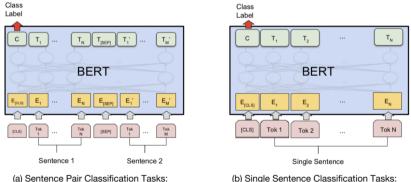


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- [CLS]: first token of all sequences; used for next sentence prediction
- Distinguish two sentences in a pair: [SEP] and segment embedding
- Learned position embedding
- 12 (base; 110M params) or 24 (large; 340M params) layer Transformer

Finetuning BERT

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

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



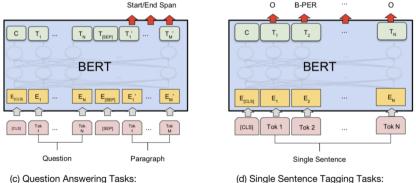
(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG (b) Single Sentence Classification Tasks: SST-2, CoLA

Finetuning BERT

SQuAD v1.1

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

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



(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.

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

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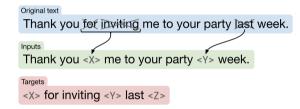
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How do we train the encoder-decoder?

- 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

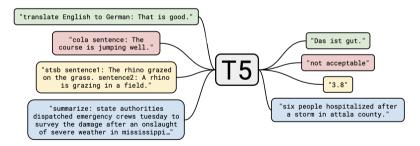


Compare with encoder-only models:

- 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

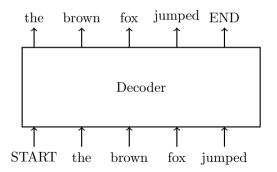
- Formulate the task in text-to-text format
- Fine-tune all parameters (similar to BERT fine-tuning)
- Advantages over encoder models: unified modeling of many different tasks including text generation

Decoder-only models

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

$$\begin{aligned} s_1, \dots, s_m &= \text{Decoder}(y_0, \dots, y_{m-1}, h_1, \dots, h_n) \\ \rho(y_i \mid y_{< i}) &= \text{softmax}(Ws_i + b) \end{aligned}$$

(A prefix of *y* can be the input.)



(more on language models later)

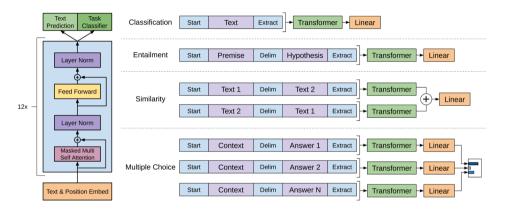
Generative Pretraining (GPT)

- 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 $L_{task} + \lambda L_{LM}$ (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 Transformer w/o aux LM LSTM w/ aux LM | 59.9 75.0 69.1 | 18.9 47.9 30.3 | 84.0 92.0 90.5 | 79.4 84.9 83.2 | 30.9 83.2 71.8 | 65.5 69.8 68.1 | 75.7 81.1 73.7 | 71.2 86.9 81.1 | 53.8 54.4 54.6 |

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

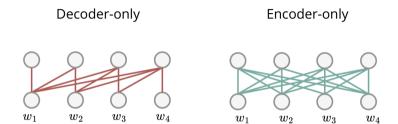
Compare with BERT

| 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 |
| BERTBASE | 84.6/83.4 | 71.2 | 90.5 | 93.5 | 52.1 | 85.8 | 88.9 | 66.4 | 79.6 |
| BERTLARGE | 86.7/85.9 | 72.1 | 92.7 | 94.9 | 60.5 | 86.5 | 89.3 | 70.1 | 82.1 |

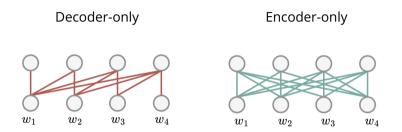
Table 1: GLUE Test results, scored by the evaluation server (https://gluebenchmark.com/leaderboard). The number below each task denotes the number of training examples. The "Average" column is slightly different than the official GLUE score, since we exclude the problematic WNLI set.⁸ BERT and OpenAI 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



Encoder-only vs decoder-only models: attention



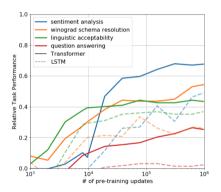
Encoder-only models provides better embeddings due to bidirectional attention.

Encoder-only vs decoder-only models: generation

Decoder-only models can make predictions through generation without finetuning

Encoder-only vs decoder-only models: generation

Decoder-only models can make predictions through generation without finetuning



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

Encoder-only vs decoder-only models: training efficiency

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What about encoder-decoder models?

- Better for sequence-to-sequence tasks
- Need to maintain two separate architectures, additional cross attention
- Overall limited advantage over decoder-only models

What are these models trained on?

Both quantity and quality are important

- Wikipedia: encyclopedia articles (clean, single domain)
- Toronto Books Corpus: e-books (diverse domain)
- WebText (40GB): content submitted to Reddit with a vote \geq 3 (diverse, bias)
- CommonCrawl (20TB): scraped HTML with markers removed (diverse, large, noisy, bias)
 - A cleaned version: C4 (750GB)

Active research area: What data is good for pretraining?

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Approaches to speed up pretraining

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Approaches to speed up pretraining

- Reduce model size
- Design more sample-efficient learning objectives
- Improve efficiency of self-attention
- Improve system-level efficiency

Idea 1: reduce the number of parameters

ALBERT (a lite BERT) [Lan et al., 2020]

Factorization:

- Recall that in Transformer, we first need to map the one-hot encoding (of size V) of a token to Q, K, V embeddings (of size H)
- The number of parameters is $V \times H$
- We can instead first map it to a lower-dim space (of size *E*) so that the number of params is $V \times E + E \times H$

Idea 1: reduce the number of parameters

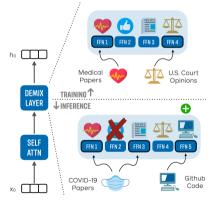
ALBERT (a lite BERT) [Lan et al., 2020]

• Parameter sharing:

- Share feedforward network weights across layers
- Share self-attention weights across layers
- ALBERT: share all params across layers

Idea 2: reduce interaction among parameters (sparse/modular architectures)

DEMix [Gururangan et al., 2022]



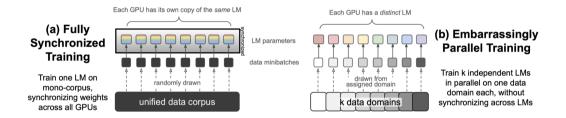
- Replace the FFN layer with an ensemble of *n* experts
- Route examples to experts corresponding to its domain determinstically

$$\operatorname{FFN}(h) = \sum_{i=1}^{n} \mathbb{I}[x \in \operatorname{\mathsf{domain}} i] \operatorname{FFN}_{i}(x)$$

• Only a subset of params are active for each example/batch

Idea 2: reduce interaction among parameters (sparse/modular architectures)

Branch-Train-Merge [Li et al., 2022]



- Train domain experts in parallel and ensemble them (or take weighted average of their parameters)
- Reduce synchronization among GPUs at the cost of increased model size
- Easy to expand/remove domain experts

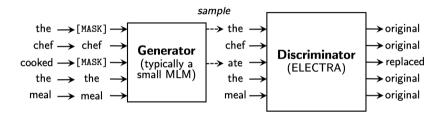
Approach 2: design sample-efficient learning objectives

ALBERT: Inter-sentence coherence loss

- Motivation: the next sentence prediction task is too easy
- Design hard negative examples
- Input: take two consecutive sentences, swap their order randomly
- Output: predict if they are in natural order *I went home. SEP I slept.* +1 *I slept. SEP I went home.* -1
- Model needs to learn temporal order of events (commonsense, causality etc.)

Approach 2: design sample-efficient learning objectives

ELECTRA [Clark et al., 2020]: discriminate from true vs guessed tokens



- First train the generator for n steps using the MLM objective.
- Freeze generator weights. Train the discriminator using the sequence classification objective. Keep discriminator for finetuning.
- Comparison with MLM: predict at every position; hard negative examples.

Approach 2: design sample-efficient learning objectives ELECTRA result:

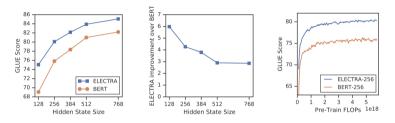


Figure: Finetuning result on the GLUE benchmark

- Larger improvement at smaller model sizes
- Faster training
- An effective approach if you don't have large compute for pretraining

Approach 3: alternatives to self-attention

Transformer recap

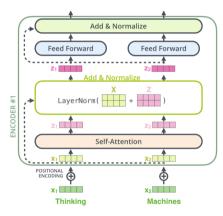


Figure: From The Illustrated Transformer

Which components require matrix multiplication?

Approach 3: alternatives to self-attention

Transformer recap

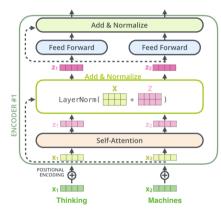


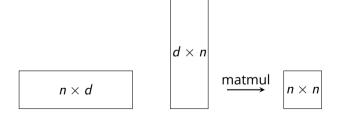
Figure: From The Illustrated Transformer Which components require matrix multiplication?

- Self-attention
 - Q,K,V projection
 - Scaled dot-product attention
- Feed-forward layer

Q, K, V projection:

$$n \times d_e$$
 $\xrightarrow{\text{linear}}$ $n \times d$

Scaled dot-product attention:

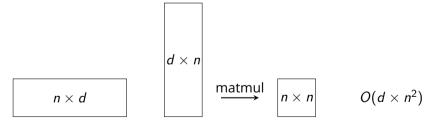


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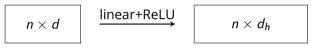
$$n \times d_e$$
 $\xrightarrow{\text{linear}}$ $n \times d$

$$O(n \times d_e \times d)$$

Scaled dot-product attention:



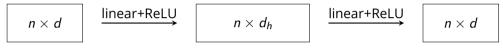
Feed-forward layer (GPT-2):



 $O(n \times d \times d_h)$

- Two-layer FFN
- $d_h = 4d (d > 1K)$ by default in GPT-2
- Approximately half of the compute time

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Improve efficiency of self-attention (for long sequences)

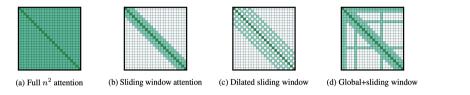
Improve efficiency of self-attention (for long sequences)

Key idea: reduce the $O(n^2)$ time and memory cost

- Sparsify the attention matrix
 - Deterministic mask
 - Data-dependent mask (Reformer [Kitaev et al., 2020])
- Compress the key-value memory
 - Low-rank projection
 - Attention-based projection

Sparse attention

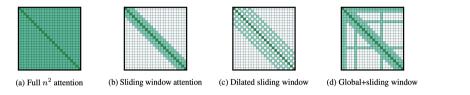
Longformer [Beltagy et al., 2020]: attention within a local window



- Sliding window: attending to a *local* window of size w around each token $O(n \times w)$
- Dilated sliding window: reaching *longer range* with a larger window size with gaps
- Global window: full attention on specific tokens, e.g., [CLS] in BERT

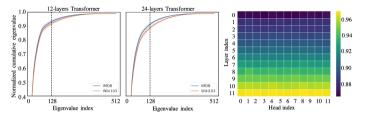
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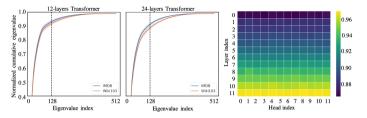


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- Dilated sliding window: reaching *longer range* with a larger window size with gaps
- Global window: full attention on specific tokens, e.g., [CLS] in BERT
- Details: balancing efficiency and performance
 - Adding dilation on some heads
 - Using small window size on lower layers and larger ones on higher layers

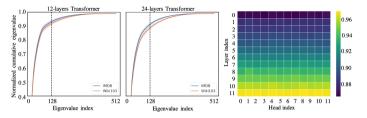
Self-attention is low rank [Wang et al., 2020]



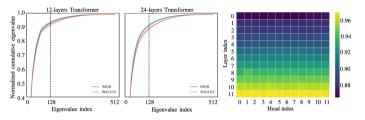
• Left: cumulative eigenvalues of pretrained transformer with n = 512



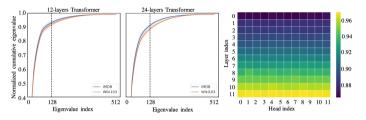
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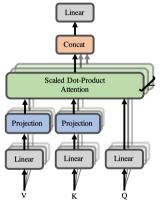


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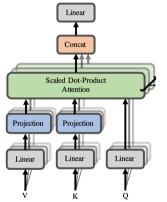
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- **Idea**: instead of attending to *n* tokens, attend to *k* principal components

Linformer [Wang et al., 2020]: compute self-attention in a lower dimension



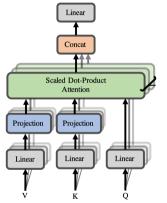
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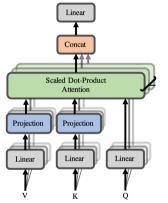


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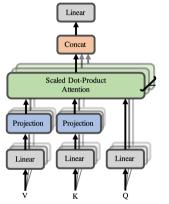
• Attend to the lower-dimensional memory: softmax $\left(Q_{n \times d} K_{k \times d}^T / \sqrt{d}\right)$



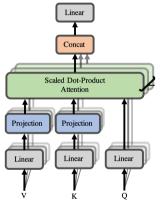
- Reduce dimensionality of the "memory": Map K, V from $n \times d$ to $k \times d$
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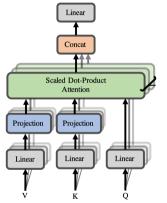
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 - Unclear how to mask: past and future are mixed

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Improve the quadratic time and space complexity of self-attention

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Bad news: Most techniques are not widely used in large pretrained models now. Why?

- Improvement in time/space complexity doesn't always translate to real time/space savings
- These techniques often breaks structure and sacrifice the batching ability on GPUs
- Only see improvement on very long sequences

Approach 4: system-level approaches

- Operates at a lower abstraction level
- Often brings more direct impact on efficiency
- Example:
 - Gradient accumulation
 - Model and data parallelism (e.g., deepspeed)
 - Flash attention: exploit GPU memory asymmetry

