

Advanced Natural Language Processing

1 LLMs

BERT

Bidirectional Encoder Representations from Transformers.

Basically a transformer encoder.

Training: BERT was trained on Books and Wikipedia.

Training objectives: Masked Language Modelling. Predict randomly masked tokens (by [MASK] token). Next Sentence Prediction (with [CLS] token).

Versions:

- BERT-Base: 12 transformer blocks, embedding dim: 768, 12 attention heads.
- BERT-Large: 24 transformer blocks, embedding dim: 1024, 16 attention heads.

Extensions:

- RoBERTa: Larger batches, removed NSP.
- SentenceBERT: BERT + siamese architecture (Sentence A and B in the same model, outputs are compared by some metric) + triplet loss (tune network such that distance between anchor sentence and positive sentence is smaller than anchor sentence and negative sentence)
- DistillBERT: Larger teacher network creates soft probability distribution labels. Smaller student model tries to replicate these distributions.

GPT

Generative Pretrained Transformer.

Only a transformer decoder, since its task is not seq2seq, where you might want to refer to another part of the input sentence, but instead just generate next tokens (still the decoder receives already generated tokens as inputs).

Goal is to use few-shot learning and prompting instead of fine-tuning and task specific architectures.

Autoregressive: Feeds back generated tokens in decoder input.

Other LLMs

T5

Text-to-Text-Transfer-Transformer.

Encoder and decoder block, similar to original Attention is all you need paper but with slight modifications.

RETRO

Retrieval-Enhanced Transformer.

Enhanced by large text database.

In total 4% of GPT-3 size.

Flash Attention

Self-attention is the bottleneck when training/inferencing transformers (quadratic time). During Attention, tensors are moved from HBM (High Bandwidth (GPU) Memory) to SRAM (Shared random-access (GPU) memory) multiple times: Before each operation, the tensors are moved from HBM to SRAM and then written back to HBM.

Flash Attention fuses multiple operations into one kernel, thus saving load and write operations. It is becoming the standard for transformers.

Approximate a complex model with a transparent one

Fine-Tuning

Traditional fine-tuning: Re-train all parameters with a small labelled dataset for example on domain knowledge.

Traditional fine-tuning with freezing: Freeze a part of the model.

Prompting

Removes the need for additional layers for a downstream task. Uses the same format as the pretraining objective of LLMs: We ask the LLM to generate the answer based on a task-specific input.

Requires no new parameter, can be practiced on a closed-source LLM.

Zero-Shot

Simple prompting is equivalent to zero-shot learning. The model predicts the answer based on the question.

Example: "Translate English to French: cheese = ".

In-Context Learning and Few-Shot Learning

Learning that contains examples of solutions to the task.

Example: "Translate English to French: sea otter = loutre de mer. cheese = ".

Prompting Terminology

Pattern:

A function that maps input to text (i.e. template for x).

Example: $f(x) = \text{"Review : } x\text{"}$

Verbalizer:

A function that maps a label to text (i.e. template for y).

Example: $v(y) = \text{"Sentiment : } y\text{"}$

Zero-shot prompting is using one pattern. Few-shot prompting is using many pairs of patterns and verbalizers and one final pattern.

Choosing a prompt is important and non-trivial, since experiments show different patterns and verbalizers exhibit large variance on the result accuracy. Additionally, it is uncertain how and why in-context learning works.

Reasons:

- Different input and output space distributions decrease/increase performance.
- LLM sees demonstrations not as ordered pairs.
- Highly dependent on choice, order and term frequency.

Prompting still works really well in practice and can perform better than smaller task-specific fine tuned models such as BERT.pretrained

Prompt-based fine tuning: [CLS] A _ master class. It was [MASK].

Parameter Efficient Fine-Tuning

Prompt Search

Learns tokens in the prompt.

Instead of fine-tuning and predicting a [CLS] token for an input sentence, use the masked prompt as input sentence.

Classical fine-tuning: [CLS] A three-hour cinema master class.

Prompt search: [CLS] A _ master class. It was [MASK].

AutoPrompt

Prompt search method.

Update tokens in the pattern using gradient-guided search.

Prompt Template: {Original sentence}[T][T][T][T][T][MASK], where T are trigger Tokens that are determined using gradient-guided search.

Example: a real joy. atmosphere alot dialoge Clone totally [MASK].

Prompt Tuning

Attaches a learnable embedding to the input pattern.

Example: [EMBED] [CLS] A _ master class. [MASK].

Goal: Learn the [EMBED] token.

BitFit

Only tunes bias in attention and linear layers.

Hypothesis: LLM does not need to learn new linguistic features, just domain knowledge.

Adapters

In the Transformer block, after each feed-forward block, add an adapter block and a skip connection.

The adapter layer is built up like an autoencoder (down- and the up-projects the input). Then, only fine tune these adapter blocks.

LoRA

Low-Rank Adaption of LLMs.

At each layer, substitute the weight update on W with an update on the low-rank decomposition of W (AB).

$$W_{finetuned} = W_{pretrained} + \Delta W = W_{pretrained} + AB$$

Low rank means the matrix has much less params than W .

(IA)3

Infused Adapter by Inhibiting and Amplifying Inner Activations.

Element-wise rescaling of model activations with a learned vector.

Separate learned vectors for each task.

Human Preference Tuning

Fine tuning is not enough to make a model fully non-harmful/friendly and performant/helpful at the same time.

Training on human preferences (rankings, scores, etc.) is not differentiable, since no mathematically differentiable function was used to calculate the scores. Therefore, no supervised learning is possible.

Instead use Reinforcement Learning.

Reinforcement Learning with Human Feedback

Create a smaller LM, the reward model, which is trained on labelled data (4 answers to a prompt ranked from best to worst).

The reward model then calculates a reward for each output of the LLM. This reward is used with the PPO algorithm to update the LLM weights.

To not overfit and let the LLM just "please" the reward model, we calculate a second loss from the LLM output and the old, frozen LLM output. This loss is added to the reward model output before being used in the PPO algorithm.

Observations:

- Smaller models get slightly worse, bigger models get even better.
- Compatible with specialized models (e.g. model for coding)
- Requires much more human annotation than fine tuning. Possible solution: Use LLMs themselves to identify bad answers (Constitutional AI/RLAIF)

RLAIF

Reinforcement Learning with AI Feedback.

Uses a constitution (Constitutional AI) instead of humans.

1. Make the model revise harmful answers according to a random principle in the constitution. Then use fine tuning with the revised answers.
2. Use an off-the-shelf LLM to rate the answers of the fine-tuned model.
3. Train a reward model on these pairs.
4. Train the final model with reinforcement learning.

DPO

Use Direct Policy Optimization instead of reinforcement learning.

Reformulates the problem into a single cross entropy loss.

So far better than PPO, but the debate is open.

2 Embeddings and XAI

Embeddings

Static Embeddings

Word2Vec, GloVe, FastText.

One embedding per word, the same for every context.

Contextual Embeddings

ELMo, BERT, GPT.

One embedding per word, different for every context.

Produced by a transformer encoder.

Subword Embeddings

Byte-Pair Encoding (BPE)

Merge characters into tokens until desired vocabulary size is reached.

Analyzing Contextual Embeddings

Goal: Find information encoded in the embedding such as about language, the world or harmfulness.

Techniques:

- Dimensionality reduction
 - Clustering
 - Probing classifier: Train a classifier to evaluate specific properties such as POS, sentiment or NER.
 - Association Tests: Use cosine similarity to measure association between two concepts and attributes A and B.
 - POLAR: Subtract two polar opposite embeddings, then multiply with the target word embedding to receive the score of that embedding in the polar opposite embedding space.
- Disadvantages: requirement of opposites and dictionaries, requirement of quality context examples (potential source of bias).

Topic Modelling

Identifying abstract themes in a collection of documents.

Old methods:

- Latent Dirichlet Allocation: Topics are characterized as a distribution over words.
- Variational autoencoders: Compression of documents to a topic distribution.

BERTopic:

Modular approach to topic modeling. Composed of six steps, each is interchangeable:

1. Generate embeddings (SBERT, spaCy, other transformers)
2. Dimensionality Reduction (PCA, UMAP, TruncatedSVD)
3. Clustering (HDBSCAN, k-means, BIRCH)
4. Tokenizer (CountVectorizer, Jieba, POS)
5. Weighting scheme (c-tf-idf, c-tf-idf + BM25, c-tf-idf + normalization)
6. (optional) Representation Tuning (ChatGPT, Llama, MMR)

2.1 Explainability and Problem Solving

Limitations:

- Multi-step reasoning is hard for LLMs, they generally greedily produce the next token
- Hallucinations: LLM data may be incorrect or outdated, LLM output always looks highly plausible.

Explainable AI (XAI) methods:

- Transparent models: Use inherently transparent models like linear regression or decision trees.
- Model-specific analysis: Fine grained analysis of small neural networks. I.e. choose a neuron in the network and watch its activation for multiple inputs.
- Model-agnostic analysis: Find patterns between model input and output
- Prompting techniques: Make the LLM thought process more transparent (Chain-of-thought)

Model-Agnostic Analysis

Surrogates: Train a simpler, smaller, transparent model that mimics the big model

Feature Attribution: Add an importance score to each feature and measure the result.

Approaches: Remove or replace tokens in a prompt, measure the gradient of output logits.

SHAP:

- Task: Predict income of a person using a set of features
- Question: What was the impact of a certain feature on the prediction?
- Step 1: Determine all combinations of features

- Step 2: Train a model for each combination and measure impact of features(s) on prediction
- Step 3: Calculate marginal contribution of each feature to the prediction
- Step 4: Interpretation

Chain-of-Thought Prompting:

Similar to few-shot learning, where an example with the thought procedure in the answer is given. Leads to better and more explainable results, but some tasks are still too difficult for Chain-of-Thought.

Tree-of-Thought:

4 Components:

- Thought Decomposition: Decompose thought into smaller, simpler thoughts
- Thought Generator: Generate candidates for the next thought step
- State Evaluator: Evaluate progress made towards problem solution
- Search Algorithm: Searching for high-value thoughts

We can now explore different continuations and evaluate them. This combines principles such as Planning, Lookahead and Backtracking.

Probabilistic Tree-of-Thoughts: Assign probabilities to answers.

3 types of question answering:

- Open-Book: Look for answers in the web or DB
- Closed-Book: LLM generates answer
- Child-aggregated: Reason about answer by looking at the child answers.

Difference from regular Tree-of-Thought: The thought decomposition into a tree is done by the LLM instead of the user. The corrections also can be enhanced by choosing from the different question answering strategies based on the assigned probabilities to the answers.

Big Problem in XAI:

Dilemma between plausibility to humans and faithfulness to the model. With our strategies we instead can let the model explain its own reasoning, which kind of solves the dilemma.

Multimodality and Multilinguality

Stable Diffusion

Add gaussian noise step by step to an image.

Use a U-Net to predict all the noise that was added to the original image from all noise steps until t . This requires conditioning the U-Net with t .

Then subtract the predicted noise from the noisy input.

Then, add back t - noise.

Repeat the steps above until $t = 0$.

At inference, take random noise as $t = T$ and condition the U-Net with the prompt.

Additionally, predict the noise without the prompt and use a divergence measure to amplify the output with the prompt.

Multilinguality

Language model as prior: Pre-trained LM's as source of prior knowledge for downstream tasks.

Deep Fusion: Goal: Translation model from HRL (High resource language) 1 to LRL, but not much data available. Solution: Train transformer on translation of HRL 1 to HRL 2, for which more data to LRL is available. Then replace the decoder with a decoder from HRL 1 to LRL.

Pivot languages: Use an intermediate language for translating a uncommon translation pair.

Seq2Seq and Evaluation

Seq2Seq

Source: Input

Reference: Desired output

Candidate: Generated output

Features of a good Seq2Seq output:

- Fluency: Quality of target language text
- Adequacy: Preservation of exact meaning

BART:

- Trained by corrupting text with an arbitrary noise function and learning to reconstruct the original text
- Mix of Bidirectional Encoder (BERT) and Autoregressive Decoder (GPT)

Advantage of Seq2Seq: Cross-attention shows influence of input tokens on output tokens.

XAI for free.

PEGASUS:

- Pre-training objective for abstractive summarization: Gap sentence generation (GSG); generate the missing sentences

Faithfulness: Staying consistent and truthful to the source.

Hallucination: Outputs that are nonsensical or unfaithful to source.

- Intrinsic: misrepresented information contradicting source.

- Extrinsic: generating information not contained in the source.

Textual Entailment: Train a classifier that checks if generated answers are entailed in source.

Question answering for hallucination detection:

1. Extract possible answers
2. Generate questions for these answers
3. Answer question with source
4. Compare both answers

Model-based hallucination detection: Hallucinations show a different cross-attention pattern, can be measured using Wasserstein distance.

Evaluation

Human Evaluation

Evaluation of language generation is difficult.

Human evaluation is gold standard, but expensive. Human evaluation can produce many different, but correct candidates for a source, which limits reproducibility.

Reference-based Evaluation

BLEU:

- Bilingual Evaluation Understudy
- Calculates ratio of overlapping n -grams (weighted sum over different values for n)
- Add penalty for short sentences

SacreBLEU:

- Standardized version of BLEU
- Not sensitive to tokenization (punctuation, compounds)

Problems of overlap-based methods:

- No synonym awareness
- Only partially robust to word order
- Cross sentence properties are hard

BERTScore:

- Cosine similarity between contextual embeddings of reference and candidate

Problems:

- Latent representations are not always distinctive (for example for antonyms)
- Grammatical correctness not always covered
- Performance dependent on model strength

BLEURT: Bilingual Evaluation Understudy with Representations from transformers

- Pre-trained BERT with score output
- Trained on human scores
- Additional pre-training on synthetic data

COMET: Cross-lingual Optimized Metrics for Evaluation of Translations

- Pre-trained multilingual model with score output
- Trained on human scores

Learned Metrics such as BLEURT and COMET are good (best correlation with human scores) but have to be optimized for specific tasks, makes it hard to compare between papers, no one-fits-all solution

Reference-free Evaluation

Compare semantic overlap against source instead of reference.

Evaluating with LLMs: No Reference needed, can use few-shot prompting

Explainable Scores

Jointly learn sentence level score and word level annotations. The evaluation metric adds post-hoc word annotations.

INSTRUCTSCORE: Explainable score based on LLaMa.

Candidate Ranking: Models are often confident with their outputs. Idea: Generate multiple translation candidates and rank them with evaluation metric. Then return the highest ranking candidate.

Benchmarking LLMs

HELM (Holistic Evaluation of Language Models):

- 87 Scenarios
- Question answering
- Summarization
- Sentiment analysis
- Reasoning

Problems:

- Evaluation is usually few-shot based. Changing things like the prompt template can change model ranks.
- Data contamination: Benchmark data is open-source, models probably have learned from benchmark data. Some models can even reproduce samples from benchmarks.
- Saturation: Models already outperform humans
- Overfitting: Models train on synthetic data from GPT-4, some benchmarks are evaluated by GPT-4
- Need for multilingual benchmarks

Data, Bias and Ethics

Data

Weak Supervision

Techniques when labeled data is hard to obtain.

Approaches:

- Combination of small amount of human labeled data and a large amount of unlabeled data
- Define rules and heuristics that can label data automatically (labeling function)

Data Augmentation

- Character-, word- or sentence-level
- Synonym replacement, random shuffling
- Rephrasing, back-translation

Active Learning

1. Train model with annotated data
2. Use acquisition function to select examples from unlabeled data
3. Annotate selected data
4. Add newly labeled examples to training data, then repeat

Bias and Ethics

Data can be biased ("biased world" issue). Bias can come from the source or the way data was collected. Simple case: Class imbalance. But often detecting bias in data is hard. Its easier to detect bias in the model itself.

Detecting Bias in Systems

Association tests:

Difference between two sets of target words X and Y with respect to two sets of attribute words A and B . Cosine similarity can be used as a distance measure. The result determines if the target words X are correlated with attributes A or the targets Y are correlated with attributes B or if there is no bias.

Error analysis:

Measure bias directly from performance on test data. Good Example: Performance of NLP tasks in different languages.

Counterfactual evaluation: Manipulate test cases to change part of the input without changing the target label.

Mitigating Bias

Embedding debiasing: Bias means vector difference across unwanted dimensions. We can neutralize, equalize or soften the subspace until tests show no bias. Problem: Embedding analysis shows that bias is still encoded in the model, although not visible in the result.

Feature invariant methods: Change the training objective to penalize being able to identify protected variables.

Data Augmentation

Theoretically, one could alter input data to invert biases. The best approach but not do-able due to cost and time.

Bias Research Problems

- Vague as to who is harmed and why
- What is bias and what not
- Mismatch between problem and solutions
- Need to be more clear about what to mitigate

Conversational AI and Knowledge Enhancement

Dense Passage Retriever

Retrieve documents and passages from a corpus. Idea: Represent both query and documents in a continuous vector space.

Retrieval Augmented Generation (RAG)

Split document corpus into chunks of text and create an index.

Given a user query, compare the vector representation of that query with the document index. Select all chunks that are similar to the query and append them to the query, then feed into LLM.

Chunking

Split text into concise information pieces. Splitting is possible based on data structure (document, page, table), text structure (chapter, paragraph), content length or a learned heuristic.

Chunk boundaries are important to not lose information.

Metadata: Can be used to hard-filter. Alternatively include as text into the chunk.

A chunk is then defined as a value and a key (index).

Key: Embedding vector.

Value: The text chunk.

The same LLM is used for creating the chunk embeddings and the query embedding.

Chunk selection: Cosine similarity, selecting the top k chunks.

How to evaluate:

- Answer relevance: Reference-free methods
- Answer correctness: Reference-based
- Groundedness: Reference-free
- Context relevance: Reference-based (regular IR metrics such as recall/precision)

Painpoints of RAG:

Find questions instead of answers. Solution: Query expansion:

- Guess potential answers for a query using a LLM
- Retrieve chunks for those answers + the original query

Suboptimal chunks. Solution: Split text when topic shifts (i.e. when cosine similarity between embeddings changes)

Solution 2: Hierarchical chunking:

- Split into smaller chunks iteratively (1. split on doc structure, 2. split on semantic, 3. hierarchical splitting on text length)

Model cannot deal with non-relevant documents. Solution: Define a similarity threshold that chunks need to have to be valid context.

Lack of exact match capabilities. Solution: Hybrid Search: Vector search and keyword search.

Lost in the middle. Solution: Position crucial data at beginning or end of input context.

Adapters

Insert a small network before the residual addition in the transformer block.

Will lead to 1-8% increase in parameters.

Can train adapter with things like knowledge graph.

Pre-trained adapters can be re-used.

LoRA is sometimes still a better approach.