Introduction to Large Language Models

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Overview

- **The Next-Token Prediction Paradigm**
  - Stochastic modeling of languages
  - Conditional distribution estimation
- **The Transformer Architecture**
  - Attention mechanism: Self-attention and multi-head attention
  - Positional encoding and why it's needed
  - Layer structure: Encoder vs. decoder
- **Generative Pre-trained Transformer (GPT) Models**
  - Pretraining: Learning from large, diverse datasets
  - Fine-tuning: Specializing GPT for specific tasks
  - GPT-3 and beyond: Scaling and capabilities

Shannon's Stochastic Approximation of English

Claude E. Shannon, "A Mathematical Theory of Communication", 1948

3. THE SERIES OF APPROXIMATIONS TO ENGLISH

To give a visual idea of how this series of processes approaches a language, typical sequences in the approximations to English have been constructed and are given below. In all cases we have assumed a 27-symbol "alphabet," the 26 letters and a space.

1. Zero-order approximation (symbols independent and equiprobable).

    XFOML RXKHRJFFJUJ ZLPWCFWKCYJ FFJEYVKCQSGHYD QPAAMKBZAACIBZL-HJQD.

- "... a discrete source as generating the message, symbol by symbol. It will choose successive symbols according to certain probabilities depending..."
- Shannon also introduces the "n-gram" model, where one models the conditional probability of next word depending on its previous *n* words.

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Goal: Find an algorithm for computing the conditional distribution $P(\cdot \mid y^t)$.

Learning Language Models

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The MLE $\hat{\theta}$ is typically computed via gradient based algorithms (e.g., SGD).

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Major Architectures Include:

- **n-gram Models**: Use fixed-length context of $n - 1$ words.
- **Recurrent Neural Networks (RNNs)**: Process sequences word-by-word, capturing temporal dependencies.
- **Long Short-Term Memory (LSTM)**: A type of RNN designed to capture long-range dependencies.
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This lecture will focus entirely on the transformer-based models.

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The Transformer Architecture

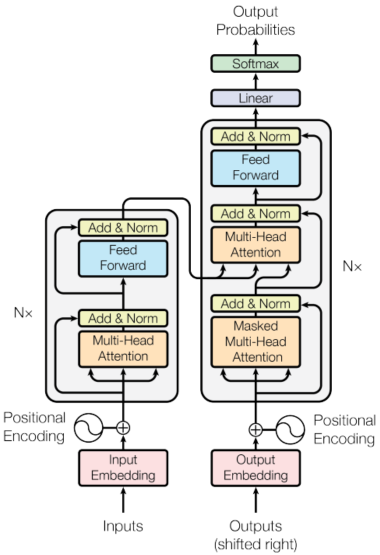

Figure 1: The Transformer - model architecture.

1. The input to the transformer is a sequence of tokens.
   - These tokens are obtained through a non-learnable tokenization process.
2. The tokens are mapped to vectors via a learnable embedding layer.
3. These vectors are combined with non-learnable positional encoding.
4. The processed vectors are passed through N repeated layers.
   - Each layer includes multi-head attention and a feed-forward MLP.
   - Each layer transforms the vectors into another of the same shape.
5. The output is a probability distribution over all possible tokens.

The Vector Embedding

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The matrix M is part of the model's parameters in a Transformer architecture and will be updated during training.

Multi-Head Attention Layer

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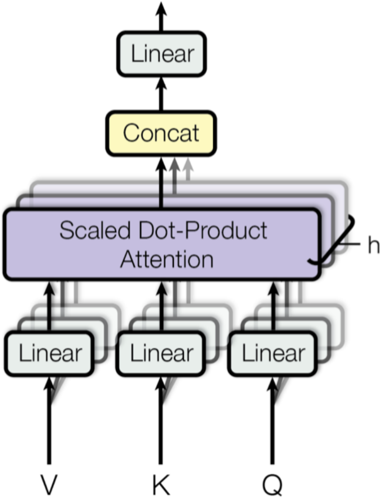

Scaled Dot-Product Attention

The attention head i transform input $X \in \mathbb{R}^{t \times d}$ into $X_i \in \mathbb{R}^{t \times d'}$ as follows:

1. Compute matrices (interpreted as query, key and value):

$$Q_i := XW_q^i, \quad K_i := XW_k^i, \quad V_i := XW_v^i, \quad \in \mathbb{R}^{t \times d'}.$$

2. Compute the scaled attention scores matrix

$$S_i := \frac{(Q_i K_i^\top)}{\sqrt{d'}} \in \mathbb{R}^{t \times t}.$$

3. Denote s_j as the jth row of S_i for $j \leq t$, which is interpreted as the attention scores for the jth token. The output is given by

$$X_i := \begin{bmatrix} \mathrm{softmax}(\mathrm{s}_1) \\ \cdots \\ \mathrm{softmax}(\mathrm{s}_t) \end{bmatrix} V_i \in \mathbb{R}^{t \times d'}$$

Here, for any $\mathbf{z} = (z_1, \cdots, z_t)$, $\mathrm{softmax}(\mathbf{z})$ corresponds to a vector $\mathbf{z}'$ such that

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Goal: the attention head map a sequence of embeddings into another sequence of the same length (t) with improved representation incorporating the context.

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The first layer computes outputs:

$$X' = \begin{bmatrix} \mathrm{ReLU}\left(\mathbf{x}_1^\top W_1 + \mathbf{b}_1^\top\right) \\ \vdots \\ \mathrm{ReLU}\left(\mathbf{x}_t^\top W_1 + \mathbf{b}_1^\top\right) \end{bmatrix} \in \mathbb{R}^{t \times d_{\mathrm{ff}}},$$

where $W_1 \in \mathbb{R}^{d \times d_{\mathrm{ff}}}$, $\mathbf{b}_1 \in \mathbb{R}^{d_{\mathrm{ff}}}$, and $\mathrm{ReLU}(x) := \max\{0, x\}$ is applied entry-wise.

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Denote $X' = [\mathbf{x}'_1, \cdots, \mathbf{x}'_t]^\top$. The final output is given by:

$$\begin{bmatrix} \mathbf{x}_1'^\top W_2 + \mathbf{b}_2^\top \\ \vdots \\ \mathbf{x}_t'^\top W_2 + \mathbf{b}_2^\top \end{bmatrix} \in \mathbb{R}^{t \times d},$$

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$$\mathbf{z}_t = \mathbf{x}_t^\top M \in \mathbb{R}^{|\mathcal{Y}|},$$

where $M \in \mathbb{R}^{d \times |\mathcal{Y}|}$ is the initial embedding matrix (weight tying is applied).

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$$\mathbf{z}_t = \mathbf{x}_t^\top M \in \mathbb{R}^{|\mathcal{Y}|},$$

where $M \in \mathbb{R}^{d \times |\mathcal{Y}|}$ is the initial embedding matrix (weight tying is applied).

The probabilities over $\mathcal{Y}$ are obtained using the softmax function:

$$P(y \mid \text{context}) = \frac{\exp(z_t[y])}{\sum_{y' \in \mathcal{Y}} \exp(z_t[y'])}.$$

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Let $P = [\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_t]^\top \in \mathbb{R}^{t \times d}$. The resulting combined embeddings are:

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The positional embeddings P can either be learned or predefined, such as with sinusoidal embeddings, where for $2k, 2k+1 \in [d]$:

$$\mathbf{p}_i[2k] = \sin\left(\frac{i}{10000^{2k/d}}\right), \quad \mathbf{p}_i[2k+1] = \cos\left(\frac{i}{10000^{2k/d}}\right).$$

Layer Normalization

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For any $j \leq t$, the layer normalization computes:

$$\mu_j = \frac{1}{d} \sum_{i=1}^{d} \mathbf{x}_j[i], \quad \sigma_j^2 = \frac{1}{d} \sum_{i=1}^{d} (\mathbf{x}_j[i] - \mu_j)^2$$

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Then, the normalized output is:

$$\mathbf{x}_j' = \gamma \odot \left(\frac{\mathbf{x}_j - \mu_j}{\sqrt{\sigma_j^2 + \epsilon}} \right) + \beta$$

where $\gamma, \beta \in \mathbb{R}^d$ are learnable parameters, and ϵ is a small constant.

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Let $S_i = \frac{Q_i K_i^\top}{\sqrt{d'}} \in \mathbb{R}^{t \times t}$ be the attention score matrix. The masked attention modifies the score matrix to

$$S_i + \underbrace{\begin{bmatrix} 0 & -\infty & -\infty & \cdots \\ 0 & 0 & -\infty & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}}_{\text{mask matrix}} \in \mathbb{R}^{t \times t},$$

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The mask matrix ensures that the attention score at each position attends only to previous tokens.

Additional Remarks

- The attention layer is the only mechanism in the Transformer that incorporates context information between different embedding positions.
- All other blocks are applied position-wise.
- Technically, there are also residual connections that add the input of each layer to its output to help prevent vanishing gradient issues.
- There are many variants of the Transformer architecture. For example, in GPT, only the decoder block is used.

Overview

- **The Next-Token Prediction Paradigm**
  - Stochastic modeling of languages
  - Conditional distribution estimation
- **The Transformer Architecture**
  - Vector embedding
  - Attention mechanism: Self-attention and multi-head attention
  - Positional encoding and why it's needed
- **Generative Pre-trained Transformer (GPT) Models**
  - Pretraining: Learning from large, diverse datasets
  - Fine-tuning: Specializing GPT for specific tasks
  - GPT-3 and beyond: Scaling and capabilities

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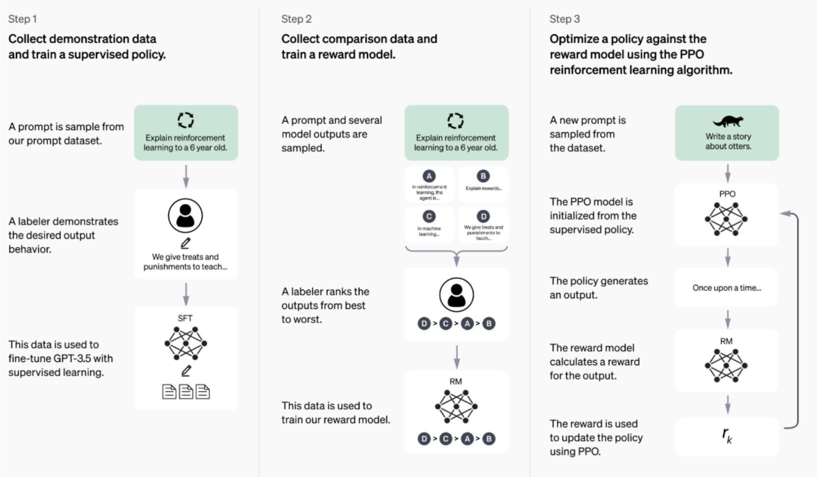
- Supervised fine-tuning, which retrains the model on a small amount of well-organized data specific to the task.
- Reinforcement Learning from Human Feedback (RLHF), which uses human annotations to train a reward model, further employed to fine-tune the original model.

Fine-tuning Pipeline of Training GPT models



Pre-training Process of GPT

Autoregressive Modeling: GPT models the probability of a sequence of tokens $y_1, y_2, \ldots, y_T$ as the product of conditional probabilities:

$$P(y_1, y_2, \ldots, y_T) = \prod_{t=1}^{T} P(y_t \mid y^{t-1}).$$

Objective: Minimize the negative log-likelihood loss over the training data $\mathcal{D} \subset \mathcal{Y}^*$:

$$\mathcal{L}(\theta) = -\frac{1}{|\mathcal{D}|} \sum_{(y_1, y_2, \ldots, y_T) \in \mathcal{D}} \sum_{t=1}^{T} \log P_\theta(y_t \mid y^{t-1})$$

where θ represents the model parameters.

Training: The model minimizes the loss $\mathcal{L}(\theta)$ by updating the parameters θ using backpropagation and gradient descent.

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$$\text{loss}(\theta) = -\mathbb{E}_{(\mathbf{x}, \mathbf{y}_w, \mathbf{y}_l) \sim \mathcal{D}} \left[\log \sigma \left(r_\theta(\mathbf{x}, \mathbf{y}_w) - r_\theta(\mathbf{x}, \mathbf{y}_l) \right) \right],$$

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Finally, the reward model is used to fine-tune a policy model using Proximal Policy Optimization (PPO).

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$$\mathsf{obj}(\phi) = \mathbb{E}_{(\mathbf{x},\mathbf{y})\sim\mathcal{D}_{\pi_\phi}}\left[r_\theta(\mathbf{x},\mathbf{y}) - \beta\log\left(\frac{\pi_\phi(\mathbf{y}\mid\mathbf{x})}{\pi^{\mathsf{SFT}}(\mathbf{y}\mid\mathbf{x})}\right)\right] - \gamma\mathbb{E}_{\mathbf{x}\sim\mathcal{D}_{\mathsf{pretrain}}}[\log(\pi_\phi(\mathbf{x}))],$$

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where:

- $\mathcal{D}_{\pi_\phi}$ is the dataset of prompts and responses generated by the current policy model π_ϕ,
- $r_\theta(\mathbf{x},\mathbf{y})$ is the reward from the reward model,
- β controls the regularization term that penalizes the KL-divergence between π_ϕ and the supervised fine-tuned policy π^{SFT}, preventing the policy from deviating too much from π^{SFT},
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PPO iteratively updates the policy π_ϕ using a gradient-based approach by sampling batches from $\mathcal{D}_{\pi_\phi}$ and $\mathcal{D}_{\mathsf{pretrain}}$.

The Scaling Law and Beyond

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Future work aims to uncover the fundamental principles governing these relationships and to identify optimal strategies for enhancing LLM performance across various domains.

There is also active research focused on understanding the undesired behaviors of LLMs, such as hallucination, and exploring the impact of alignment to mitigate these issues.

Concluding Remark

- In this lecture, we introduced the basic foundations of LLMs, from their principal objective (next token prediction), to their underlying structure (the transformer), to the training pipeline, and discussed their scalability and key challenges.
- There has been significant recent research focused on understanding the abilities of LLMs from both theoretical and empirical perspectives.
- We hope this lecture has provided readers with the basic knowledge of this rapidly evolving field.