Introduction to Large Language Models
Language models

• Remember the simple n-gram language model
  • Assigns probabilities to sequences of words
  • Generate text by sampling possible next words
  • Is trained on counts computed from lots of text

• Large language models are similar and different:
  • Assigns probabilities to sequences of words
  • Generate text by sampling possible next words
  • **Are trained by learning to guess the next word**
Large language models

• Even through pretrained only to predict words
• Learn a lot of useful language knowledge
• Since training on a lot of text
Three architectures for large language models

Decoders
GPT, Claude, Llama, Mixtral

Encoders
BERT family, HuBERT

Encoder-decoders
Flan-T5, Whisper

Pretraining for three types of architectures
The neural architecture influences the type of pretraining, and natural use cases.

Decoders
• Language models! What we've seen so far.
• Nice to generate from; can't condition on future words

Encoders
• Gets bidirectional context – can condition on future!
• How do we train them to build strong representations?

Encoder-decoders
• Good parts of decoders and encoders?
• What's the best way to pretrain them?
Encoders

Many varieties!

- Popular: Masked Language Models (MLMs)
- BERT family

- Trained by predicting words from surrounding words on both sides
- Are usually finetuned (trained on supervised data) for classification tasks.
Encoder-Decoders

- Trained to map from one sequence to another
- Very popular for:
  - machine translation (map from one language to another)
  - speech recognition (map from acoustics to words)
Introduction to Large Language Models
Large Language Models: What tasks can they do?
Big idea

Many tasks can be turned into tasks of predicting words!
This lecture: decoder-only models

Also called:

• Causal LLMs
• Autoregressive LLMs
• Left-to-right LLMs
• Predict words left to right
Conditional Generation: Generating text conditioned on previous text!

Prefix Text

Completion Text

So long and thanks for all the...
Many practical NLP tasks can be cast as word prediction!

Sentiment analysis: “I like Jackie Chan”

1. We give the language model this string:
   The sentiment of the sentence "I like Jackie Chan" is:

2. And see what word it thinks comes next:

   \[ P(\text{positive}|\text{The sentiment of the sentence ‘‘I like Jackie Chan' is:}) \]
   \[ P(\text{negative}|\text{The sentiment of the sentence ‘‘I like Jackie Chan' is:}) \]
Framing lots of tasks as conditional generation

QA: “Who wrote The Origin of Species”

1. We give the language model this string:
   
   Q: Who wrote the book “The Origin of Species”? A:

2. And see what word it thinks comes next:

   \[ P(w|Q: \text{Who wrote the book “The Origin of Species”? A:)} \]

3. And iterate:

   \[ P(w|Q: \text{Who wrote the book “The Origin of Species”? A: Charles}) \]
Summarization

The only thing crazier than a guy in snowbound Massachusetts boxing up the powdery white stuff and offering it for sale online? People are actually buying it. For $89, self-styled entrepreneur Kyle Waring will ship you 6 pounds of Boston-area snow in an insulated Styrofoam box – enough for 10 to 15 snowballs, he says.

But not if you live in New England or surrounding states. “We will not ship snow to any states in the northeast!” says Waring’s website, ShipSnowYo.com. “We’re in the business of expunging snow!”

His website and social media accounts claim to have filled more than 133 orders for snow – more than 30 on Tuesday alone, his busiest day yet. With more than 45 total inches, Boston has set a record this winter for the snowiest month in its history. Most residents see the huge piles of snow choking their yards and sidewalks as a nuisance, but Waring saw an opportunity.

According to Boston.com, it all started a few weeks ago, when Waring and his wife were shoveling deep snow from their yard in Manchester-by-the-Sea, a coastal suburb north of Boston. He joked about shipping the stuff to friends and family in warmer states, and an idea was born. [...]
The only idea was born. tl;dr Kyle Waring will...
Large Language Models: What tasks can they do?
Sampling for LLM Generation
Decoding and Sampling

This task of choosing a word to generate based on the model’s probabilities is called **decoding**.

The most common method for decoding in LLMs: **sampling**.

Sampling from a model’s distribution over words:

- choose random words according to their probability assigned by the model.

After each token we’ll sample words to generate according to their probability *conditioned on our previous choices*,

- A transformer language model will give the probability
Random sampling

\[
i \leftarrow 1 \\
w_i \sim p(w) \\
\textbf{while} \; w_i \neq \text{EOS} \\
i \leftarrow i + 1 \\
w_i \sim p(w_i | w_{<i})
\]
Random sampling doesn't work very well

Even though random sampling mostly generate sensible, high-probable words,
There are many odd, low-probability words in the tail of the distribution
Each one is low-probability but added up they constitute a large portion of the distribution
So they get picked enough to generate weird sentences
Factors in word sampling: **quality** and **diversity**

Emphasize **high-probability** words
+ **quality**: more accurate, coherent, and factual,
- **diversity**: boring, repetitive.

Emphasize **middle-probability** words
+ **diversity**: more creative, diverse,
- **quality**: less factual, incoherent
Top-k sampling:

1. Choose # of words \( k \)
2. For each word in the vocabulary \( V \), use the language model to compute the likelihood of this word given the context \( p(w_t | w_{<t}) \)
3. Sort the words by likelihood, keep only the top \( k \) most probable words.
4. Renormalize the scores of the \( k \) words to be a legitimate probability distribution.
5. Randomly sample a word from within these remaining \( k \) most-probable words according to its probability.
Top-p sampling (= nucleus sampling)

Holtzman et al., 2020

Problem with top-k: $k$ is fixed so may cover very different amounts of probability mass in different situations

Idea: Instead, keep the top $p$ percent of the probability mass

Given a distribution $P(w_t | w_{<t})$, the top-$p$ vocabulary $V(p)$ is the smallest set of words such that

$$
\sum_{w \in V(p)} P(w | w_{<t}) \geq p
$$
Temperature sampling

Reshape the distribution instead of truncating it

Intuition from thermodynamics,
- a system at high temperature is flexible and can explore many possible states,
- a system at lower temperature is likely to explore a subset of lower energy (better) states.

In low-temperature sampling, \( \tau \leq 1 \) we smoothly
- increase the probability of the most probable words
- decrease the probability of the rare words.
Temperature sampling

Divide the logit by a temperature parameter $\tau$ before passing it through the softmax.

Instead of

$$ y = \text{softmax}(u) $$

We do

$$ y = \text{softmax}(u/\tau) $$
Temperature sampling \[ 0 \leq \tau \leq 1 \]

\[
y = \text{softmax}(u/\tau)
\]

Why does this work?

- When \( \tau \) is close to 1 the distribution doesn’t change much.
- The lower \( \tau \) is, the larger the scores being passed to the softmax.
- Softmax pushes high values toward 1 and low values toward 0.
- Large inputs pushes high-probability words higher and low probability word lower, making the distribution more greedy.
- As \( \tau \) approaches 0, the probability of most likely word approaches 1.
Sampling for LLM Generation
Pretraining Large Language Models: Algorithm
Pretraining

The big idea that underlies all the amazing performance of language models

First **pretrain** a transformer model on enormous amounts of text

Then **apply** it to new tasks.
Self-supervised training algorithm

We just train them to predict the next word!

1. Take a corpus of text
2. At each time step $t$
   i. ask the model to predict the next word
   ii. train the model using gradient descent to minimize the error in this prediction

"Self-supervised" because it just uses the next word as the label!
Intuition of language model training: loss

- **Same loss function: cross-entropy loss**
  - We want the model to assign a high probability to true word $w$
  - $= \text{want loss to be high if the model assigns too low a probability to } w$
- **CE Loss:** The negative log probability that the model assigns to the true next word $w$
  - If the model assigns too low a probability to $w$
  - We move the model weights in the direction that assigns a higher probability to $w$
Cross-entropy loss for language modeling

**CE loss**: difference between the correct probability distribution and the predicted distribution

\[
L_{CE} = - \sum_{w \in V} y_t[w] \log \hat{y}_t[w]
\]

The correct distribution \(y_t\) knows the next word, so is 1 for the actual next word and 0 for the others.

So in this sum, all terms get multiplied by zero except one: the log \(p\) the model assigns to the correct next word, so:

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

- At each token position $t$, model sees correct tokens $w_{1:t}$,
  - Computes loss ($-\log$ probability) for the next token $w_{t+1}$
- At next token position $t+1$ we ignore what model predicted for $w_{t+1}$
  - Instead we take the **correct** word $w_{t+1}$, add it to context, move on
Training a transformer language model

Loss

Language Modeling Head

Stacked Transformer Blocks

Input Encoding

Input tokens

So long and thanks for all

Next token

log \( y_{\text{long}} \)
log \( y_{\text{and}} \)
log \( y_{\text{thanks}} \)
log \( y_{\text{for}} \)
log \( y_{\text{all}} \)

\[ \text{Loss} = \frac{1}{T} \sum_{t=1}^{T} L_{CE} \]
Pretraining Large Language Models: Algorithm
Pretraining data for LLMs
LLMs are mainly trained on the web

Common crawl, snapshots of the entire web produced by the non-profit Common Crawl with billions of pages

Colossal Clean Crawled Corpus (C4; Raffel et al. 2020), 156 billion tokens of English, filtered

What's in it? Mostly patent text documents, Wikipedia, and news sites
The Pile: a pretraining corpus

The core contributions of this paper are:

1. The introduction of a 825.18 GB English-language dataset for language modeling combining 22 diverse sources.

2. The introduction of 14 new language modeling datasets, which we expect to be of independent interest to researchers.

3. Evaluations demonstrating significant improvements across many domains by GPT-2-sized models trained on this new dataset, compared to training on CC-100 and raw Common Crawl.

4. The investigation and documentation of this dataset, which we hope will better inform researchers about how to use it as well as motivate them to undertake similar investigations of their own data.

The Pile Datasets

The Pile is composed of 22 constituent sub-datasets, as shown in Table 1. Following Brown et al. (2020), we increase the weights of higher quality components, with certain high-quality datasets such as Wikipedia being seen up to 3 times (“epochs”) for

Filtering for quality and safety

Quality is subjective

• Many LLMs attempt to match Wikipedia, books, particular websites
• Need to remove boilerplate, adult content
• Deduplication at many levels (URLs, documents, even lines)

Safety also subjective

• Toxicity detection is important, although that has mixed results
• Can mistakenly flag data written in dialects like African American English
What does a model learn from pretraining?

- There are canines everywhere! One dog in the front room, and two **dogs**
- It wasn't just big it was **enormous**
- The author of "A Room of One's Own" is Virginia **Woolf**
- The doctor told me that **he**
- The square root of 4 is **2**
Big idea

Text contains enormous amounts of knowledge. Pretraining on lots of text with all that knowledge is what gives language models their ability to do so much.
But there are problems with scraping from the web

**Copyright**: much of the text in these datasets is copyrighted
  - Not clear if fair use doctrine in US allows for this use
  - This remains an open legal question

**Data consent**
  - Website owners can indicate they don't want their site crawled

**Privacy**:
  - Websites can contain private IP addresses and phone numbers
Pretraining data for LLMs
Finetuning
Finetuning for daptation to new domains

What happens if we need our LLM to work well on a domain it didn't see in pretraining?

Perhaps some specific medical or legal domain?

Or maybe a multilingual LM needs to see more data on some language that was rare in pretraining?
Finetuning

Pretraining Data

Pretraining

Pretrained LM

Fine-tuning Data

Fine-tuning

Fine-tuned LM
"Finetuning" means 4 different things

We'll discuss 1 here, and 3 in later lectures

In all four cases, finetuning means:

taking a pretrained model and further adapting some or all of its parameters to some new data
1. Finetuning as "continued pretraining" on new data

• Further train all the parameters of model on new data
  • using the same method (word prediction) and loss function (cross-entropy loss) as for pretraining.
  • as if the new data were at the tail end of the pretraining data
• Hence sometimes called **continued pretraining**
Large Language Models

Finetuning
Evaluating Large Language Models
Perplexity

Just as for n-gram grammars, we use perplexity to measure how well the LM predicts unseen text.

The perplexity of a model $\theta$ on an unseen test set is the inverse probability that $\theta$ assigns to the test set, normalized by the test set length.

For a test set of $n$ tokens $w_{1:n}$ the perplexity is:

$$
\text{Perplexity}_\theta(w_{1:n}) = P_\theta(w_{1:n})^{-\frac{1}{n}}
$$

$$
= \sqrt[n]{\frac{1}{P_\theta(w_{1:n})}}
$$
Why perplexity instead of raw probability of the test set?

- Probability depends on size of test set
  - Probability gets smaller the longer the text
  - Better: a metric that is per-word, normalized by length

- **Perplexity** is the inverse probability of the test set, normalized by the number of words
  (The inverse comes from the original definition of perplexity from cross-entropy rate in information theory)

Probability range is [0,1], perplexity range is [1,∞]
Perplexity

- The higher the probability of the word sequence, the lower the perplexity.
- Thus the lower the perplexity of a model on the data, the better the model.
- **Minimizing perplexity is the same as maximizing probability**

Also: perplexity is sensitive to length/tokenization so best used when comparing LMs that use the same tokenizer.
Many other factors that we evaluate, like:

**Size**
Big models take lots of GPUs and time to train, memory to store

**Energy usage**
Can measure kWh or kilograms of CO2 emitted

**Fairness**
Benchmarks measure gendered and racial stereotypes, or decreased performance for language from or about some groups.
Dealing with Scale
Scaling Laws

LLM performance depends on

- Model size: the number of parameters not counting embeddings
- Dataset size: the amount of training data
- Compute: Amount of compute (in FLOPS or etc)

Can improve a model by adding parameters (more layers, wider contexts), more data, or training for more iterations.

The performance of a large language model (the loss) scales as a power-law with each of these three.
Scaling Laws

Loss $L$ as a function of # parameters $N$, dataset size $D$, compute budget $C$ (if other two are held constant)

\[
L(N) = \left( \frac{N_c}{N} \right)^{\alpha_N}
\]

\[
L(D) = \left( \frac{D_c}{D} \right)^{\alpha_D}
\]

\[
L(C) = \left( \frac{C_c}{C} \right)^{\alpha_C}
\]

Scaling laws can be used early in training to predict what the loss would be if we were to add more data or increase model size.
Large language models are large. For example the Llama 3.1 405B Instruct model from Meta has 405 billion parameters (126 layers, a model dimensionality of 16,384, 128 attention heads) and was trained on 15.6 terabytes of text tokens (Llama Team, 2024), using a vocabulary of 128K tokens. So there is a lot of research on understanding how LLMs scale, and especially how to implement them given limited resources.

In the next few sections we discuss how to think about scale (the concept of scaling laws), and important techniques for getting language models to work efficiently, such as the KV cache and parameter-efficient fine tuning.

10.5.1 Scaling laws

The performance of large language models has shown to be mainly determined by 3 factors: model size (the number of parameters not counting embeddings), dataset size (the amount of training data), and the amount of compute used for training. That is, we can improve a model by adding parameters (adding more layers or having wider contexts or both), by training on more data, or by training for more iterations. The relationships between these factors and performance are known as scaling laws. Roughly speaking, the performance of a large language model (the loss) scales as a power-law with each of these three properties of model training.

For example, Kaplan et al. (2020) found the following three relationships for loss $L$ as a function of the number of non-embedding parameters $N$, the dataset size $D$, and the compute budget $C$, for models training with limited parameters, dataset, or compute budget, if in each case the other two properties are held constant:

\[
L(N) = N^{c_N} \times N^{a_N}(10.9)
\]

\[
L(D) = D^{c_D} \times D^{a_D}(10.10)
\]

\[
L(C) = C^{c_C} \times C^{a_C}(10.11)
\]

The number of (non-embedding) parameters $N$ can be roughly computed as follows (ignoring biases, and with $d$ as the input and output dimensionality of the model, $d_{attn}$ as the self-attention layer size, and $d_{ff}$ the size of the feedforward layer):

\[
N \approx 2d n_{layer}(2d_{attn} + d_{ff})
\]

\[
\approx 12 n_{layer} d^2
\]

(assuming $d_{attn} = d_{ff}/4 = d$)

Thus GPT-3, with $n = 96$ layers and dimensionality $d = 12288$, has $12 \times 96 \times 12288^2 \approx 175$ billion parameters.
**KV Cache**

In training, we can compute attention very efficiently in parallel:

\[
A = \text{softmax} \left( \frac{QK^T}{\sqrt{d_k}} \right) V
\]

But not at inference! We generate the next tokens **one at a time**!

For a new token \( x \), need to multiply by \( W^Q \), \( W^K \), and \( W^V \) to get query, key, values

But don't want to **recompute** the key and value vectors for all the prior tokens \( x_{<i} \)

Instead, store key and value vectors in memory in the KV cache, and then we can just grab them from the cache
KV Cache

\[
\begin{align*}
\begin{bmatrix}
Q \\
q^1 \\
q^2 \\
q^3 \\
q^4 \\
\end{bmatrix} 	imes \\
\begin{bmatrix}
K^T \\
\end{bmatrix} &= \\
\begin{bmatrix}
q^1 \cdot k^1 & q^1 \cdot k^2 & q^1 \cdot k^3 & q^1 \cdot k^4 \\
q^2 \cdot k^1 & q^2 \cdot k^2 & q^2 \cdot k^3 & q^2 \cdot k^4 \\
q^3 \cdot k^1 & q^3 \cdot k^2 & q^3 \cdot k^3 & q^3 \cdot k^4 \\
q^4 \cdot k^1 & q^4 \cdot k^2 & q^4 \cdot k^3 & q^4 \cdot k^4 \\
\end{bmatrix} \\
&= \\
\begin{bmatrix}
Q \cdot K^T \\
\end{bmatrix} \\
\begin{bmatrix}
V \\
v^1 \\
v^2 \\
v^3 \\
v^4 \\
\end{bmatrix} 	imes \\
\begin{bmatrix}
V \\
v^1 \\
v^2 \\
v^3 \\
v^4 \\
\end{bmatrix} &= \\
\begin{bmatrix}
a^1 \\
a^2 \\
a^3 \\
a^4 \\
\end{bmatrix} \\
\begin{bmatrix}
Q \\
q^4 \\
\end{bmatrix} 	imes \\
\begin{bmatrix}
K^T \\
\end{bmatrix} &= \\
\begin{bmatrix}
q^4 \cdot k^1 & q^4 \cdot k^2 & q^4 \cdot k^3 & q^4 \cdot k^4 \\
\end{bmatrix} \\
&= \\
\begin{bmatrix}
Q \cdot K^T \\
q^4 \\
\end{bmatrix} \\
\begin{bmatrix}
V \\
v^1 \\
v^2 \\
v^3 \\
v^4 \\
\end{bmatrix} 	imes \\
\begin{bmatrix}
V \\
v^1 \\
v^2 \\
v^3 \\
v^4 \\
\end{bmatrix} &= \\
\begin{bmatrix}
a^4 \\
\end{bmatrix}
\end{align*}
\]
Parameter-Efficient Finetuning

Adapting to a new domain by continued pretraining (finetuning) is a problem with huge LLMs.
• Enormous numbers of parameters to train
• Each pass of batch gradient descent has to backpropagate through many many huge layers.
• Expensive in processing power, in memory, and in time.

Instead, **parameter-efficient fine tuning** (PEFT)
• Efficiently select a subset of parameters to update when finetuning.
• E.g., freeze some of the parameters (don’t change them),
• And only update some a few parameters.
LoRA (Low-Rank Adaptation)

• Transformers have many dense matrix multiply layers
  • Like $W^Q$, $W^K$, $W^V$, $W^O$ layers in attention
• Instead of updating these layers during finetuning,
  • Freeze these layers
  • Update a low-rank approximation with fewer parameters.
LoRA

• Consider a **matrix** $W$ (shape $[N \times d]$) that needs to be updated during finetuning via gradient descent.
  • Normally updates are $\Delta W$ (shape $[N \times d]$)
• In LoRA, we freeze $W$ and update instead a low-rank decomposition of $W$:
  • A of shape $[N \times r]$,
  • B of shape $[r \times d]$, $r$ is very small (like 1 or 2)
  • That is, during finetuning we update A and B instead of $W$.
  • Replace $W + \Delta W$ with $W + BA$.

Forward pass: instead of

$$h = xW$$

We do

$$h = xW + xAB$$
LoRA

Pretrained Weights

$W$

d
k

$h_1$

$1$

$X$

$d$

$X$

$r$

$k$

$A$

$B$

$d$

$r$

$k$

$x$

$d$
Large Language Models

Dealing with Scale
Harms of Large Language Models
Chatbots May ‘Hallucinate’ More Often Than Many Realize

What Can You Do When A.I. Lies About You?

People have little protection or recourse when the technology creates and spreads falsehoods about them.

Air Canada loses court case after its chatbot hallucinated fake policies to a customer

The airline argued that the chatbot itself was liable. The court disagreed.
Authors Sue OpenAI Claiming Mass Copyright Infringement of Hundreds of Thousands of Novels

The Times Sues OpenAI and Microsoft Over A.I. Use of Copyrighted Work

Millions of articles from The New York Times were used to train chatbots that now compete with it, the lawsuit said.
Privacy

How Strangers Got My Email Address From ChatGPT’s Model
Toxicity and Abuse

The New AI-Powered Bing Is Threatening Users.

Cleaning Up ChatGPT Takes Heavy Toll on Human Workers

Contractors in Kenya say they were traumatized by effort to screen out descriptions of violence and sexual abuse during run-up to OpenAI’s hit chatbot
Chatbots are generating false and misleading information about U.S. elections
Large Language Models

Harms of Large Language Models