



Introduction to Large Language Models

From Foundation to Real World Applications

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Current Trends in Theoretical Chemistry (CTTC-2024)



Agenda

Introduction

Large Language Models

Prompt Engineering

In Context Learning

Model Training

Applications

Conclusions



Introduction

OpenAI

GPT 3.5, GPT 4,
GPT 4o, GPT o1

API

Anthropic

Claude 3,
Claude 3.5

API

Google

Gemini 1,
Gemini 1.5

API

Meta

Llama 2, Llama 3,
Llama 3.1

Open Source

Mistral AI

Mixtral 8x22B,
Mistral Large 2

Open Source

Google

Gemma,
Gemma 2


Open Source

Large Language Models

- Next word or token prediction
 - I love ice ?????.
- Natural Language Processing (NLP)
 - Understand, Interpret, and Generate human language
- Large number of parameters
 - ChatGPT-4 – ~1.8 Trillion parameters
- Trained using large amount of dataset
 - ChatGPT-4 – 570 GB or 300 Billion words



Large Language Models

- 
- Model name
 - Company
 - Access
 - Number of parameters
 - Context size
 - LLM type
- Llama 3.1 405B Instruct
 - Meta
 - Open source
 - 405 Billion parameters
 - 128,000 (128K) tokens
 - Instruction fine-tuned

Sentiment Analysis

Identify sentiment of following sentence as either positive or negative.

I like "Harry Potter and the Goblet of Fire" book very much.

The sentiment of the sentence "I like 'Harry Potter and the Goblet of Fire' book very much" is Positive.

The word "like" and the phrase "very much" both indicate a strong positive sentiment, suggesting that the speaker has a very positive opinion of the book.

Summarization

Summarize the following paragraph.

A chemical reaction is a process that leads to the chemical transformation of one set of chemical substances to another. When chemical reactions occur, the atoms are rearranged and the reaction is accompanied by an energy change as new products are generated. Classically, chemical reactions encompass changes that only involve the positions of electrons in the forming and breaking of chemical bonds between atoms, with no change to the nuclei (no change to the elements present), and can often be described by a chemical equation.

A chemical reaction transforms one set of substances into another by rearranging atoms and changing energy levels. This process typically involves changes in electron positions and chemical bonds without altering the elements themselves, and is often represented by a chemical equation.

Machine Translation

Translate following English sentences in Hindi sentences.

A chemical reaction transforms one set of substances into another by rearranging atoms and changing energy levels. This process typically involves changes in electron positions and chemical bonds without altering the elements themselves, and is often represented by a chemical equation.

एक रासायनिक प्रतिक्रिया एक सेट पदार्थों को दूसरे में बदल देती है, जिसमें परमाणुओं को पुनर्व्यवस्थापन और ऊर्जा स्तरों में बदलाव शामिल होता है। इस प्रक्रिया में आमतौर पर इलेक्ट्रॉनों की स्थितियों और रासायनिक बंधनों में परिवर्तन होता है, बिना तत्वों को बदले हुए, और इसे अक्सर रासायनिक समीकरण द्वारा दर्शाया जाता है।

Creative Writing

**Write a story on chemical bond
for fifth standard student.**

The Story of Chemical Bond

Once upon a time, in a world made up of tiny particles called atoms, there lived two friends named Hydrogen and Oxygen.

...

The Moral of the Story

Chemical bonds are like friendships between atoms.

...

So, the next time you see a glass of water, remember Hydrogen and Oxygen, the two friends who formed a chemical bond to become a single molecule, Water.

***Meta-Llama-3.1-8B-Instruct**

Education and Training

In six sentences, explain the role of catalyst to first standard student.

Here's an explanation of the role of a catalyst that a first standard student can understand:

A catalyst is a special helper that makes a chemical reaction happen faster. It's like a friend who helps you build a tower with blocks, but they don't build it by themselves. The catalyst doesn't change the blocks or the tower, it just helps you build it faster. Imagine you're trying to mix two colours of paint together, but it's hard to get them to mix. A catalyst is like a special tool that helps the paint mix together quickly and easily. It's a helper that makes things happen faster and easier!

***Meta-Llama-3.1-8B-Instruct**

Education and Training

In six sentences, explain the role of catalyst to fifth standard student.

Here's an explanation of the role of a catalyst that a fifth standard student can understand:

A catalyst is a special helper that makes a chemical reaction happen faster. It's like a tool that helps mix two things together, but it doesn't change the things themselves. The catalyst helps the reaction happen by making it easier for the things to mix together. For example, in a car engine, a catalyst helps convert bad air into good air, making the engine run better. The catalyst doesn't get used up in the process, it just helps the reaction happen faster. It's like a special assistant that makes things happen more quickly and easily!

***Meta-Llama-3.1-8B-Instruct**

Education and Training

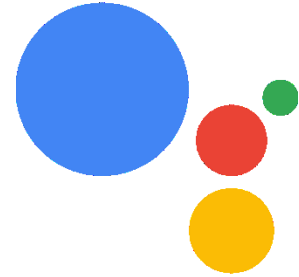
In six sentences, explain the role of catalyst to tenth standard student.

Here's an explanation of the role of a catalyst that a tenth standard student can understand:

A catalyst is a substance that speeds up a chemical reaction without being consumed or altered in the process. It's like a key that unlocks the reaction, allowing it to happen faster and more efficiently. The catalyst works by lowering the activation energy required for the reaction to occur, making it easier for the reactants to convert into products. This means that the catalyst doesn't change the reaction itself, but rather helps it happen faster. For example, in a car engine, a catalyst is used to convert pollutants into harmless gases, making the engine run more efficiently. The catalyst plays a crucial role in many industrial and biological processes, and its use can have a significant impact on the environment and our daily lives.




Virtual Assistants

- Simulate human like conversations
- Answer questions
- Provide information
- Complete simple tasks





Prompt Engineering

- Prompt
 - Inference
 - Completion
- 
- 
- 

Prompt

- Instructions to LLM
- Context for Question
- Question

Answer following question using given context.

Context: A chemical reaction transforms one set of substances into another by rearranging atoms and changing energy levels. When chemical reactions occur, the atoms are rearranged and the reaction is accompanied by an energy change as new products are generated.

Question: What is a chemical reaction?

Inference

- Large Language Model
- Model prediction

Translate following English sentences in Hindi sentences.

A chemical reaction transforms one set of substances into another by rearranging atoms and changing energy levels.

एक रासायनिक प्रतिक्रिया एक सेट पदार्थों को दूसरे में बदल देती है, जिसमें परमाणुओं को पुनर्व्यवस्थापन और ऊर्जा स्तरों में बदलाव शामिल होता है।

Prompt Completion

- Inference without context

एक रासायनिक प्रतिक्रिया एक सेट पदार्थों को दूसरे में बदल देती है, जिसमें परमाणुओं का पुनर्व्यवस्थापन और ऊर्जा स्तरों में बदलाव शामिल होता है।

In Context Learning

- Context window
- Task example/s
- Zero shot inference
- One shot inference
- Few shot inference



Context Window

- Window size
 - ChatGPT 4 Turbo – 128K
 - Llama 3.1 405B – 128K

Answer following question using given context.

Context: A chemical reaction transforms one set of substances into another by rearranging atoms and changing energy levels. When chemical reactions occur, the atoms are rearranged and the reaction is accompanied by an energy change as new products are generated.

Question: What is a chemical reaction?

Task Examples

- One or more examples
- In context learning
- Align LLM with task

Identify sentiment of following sentence as either positive or negative.

Sentence: I like book very much.

Sentiment: Positive

Sentence: I do not like book.

Sentiment: Negative

Sentence: Harry Potter and the Goblet of Fire book is good for readers.

***Meta-Llama-3.1-8B-Instruct**

Zero Shot Inference

- No examples

Identify sentiment of following sentence as either positive or negative.

Sentence: Harry Potter and the Goblet of Fire book is good for readers.

One Shot Inference

- One example

Identify sentiment of following sentence as either positive or negative.

Sentence: I like book very much.

Sentiment: Positive

Sentence: Harry Potter and the Goblet of Fire book is good for readers.

Few Shot Inference

- Two or more examples

Identify sentiment of following sentence as either positive or negative.

Sentence: I like book very much.

Sentiment: Positive

Sentence: I do not like book.

Sentiment: Negative

...

Sentence: Harry Potter and the Goblet of Fire book is good for readers.

Training Large Language Models

1

- Model pre-training
- Self supervised learning

2

- Instruction Fine Tuning
- Supervised learning

3

- Reinforcement Learning with Human Feedback
- Reinforcement learning

Retrieval Augmented Generation

- **Retrieval**

- Retrieve relevant information from database

- **Augmented**

- Retrieved information + LLM based Generation

- **Generation**

- Generate answer using LLM



Retrieval Augmented Generation

- Improve accuracy
 - Closed book test v/s Open book text with Index page
- Increase transparency
 - Text references – Retrieved documents
- Reduce hallucination
 - Augmentation – Retrieval + Generation
- Up to date information
 - Ingest documents – No expensive model training



Sahaayak – Retrieval Augmented Generation

Document Sources



Load Sources

XXXXXX XXXXX
XXXXXX XXXXX

XXXXXX XXXXX
XXXXXX XXXXX

XXXXXX XXXXX
XXXXXX XXXXX

XXXXXX XXXXX
XXXXXX XXXXX

Transform Sources

XXXXXX XXXXX
XXXXXX XXXXX

XXXXXX XXXXX
XXXXXX XXXXX

XXXXXX XXXXX
XXXXXX XXXXX

XXXXXX XXXXX
XXXXXX XXXXX

Compute Embeddings

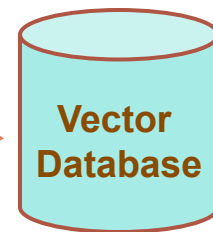
{0.25, 0.12,
0.56, 0.78}

{0.46, 0.23,
0.79, 0.68}

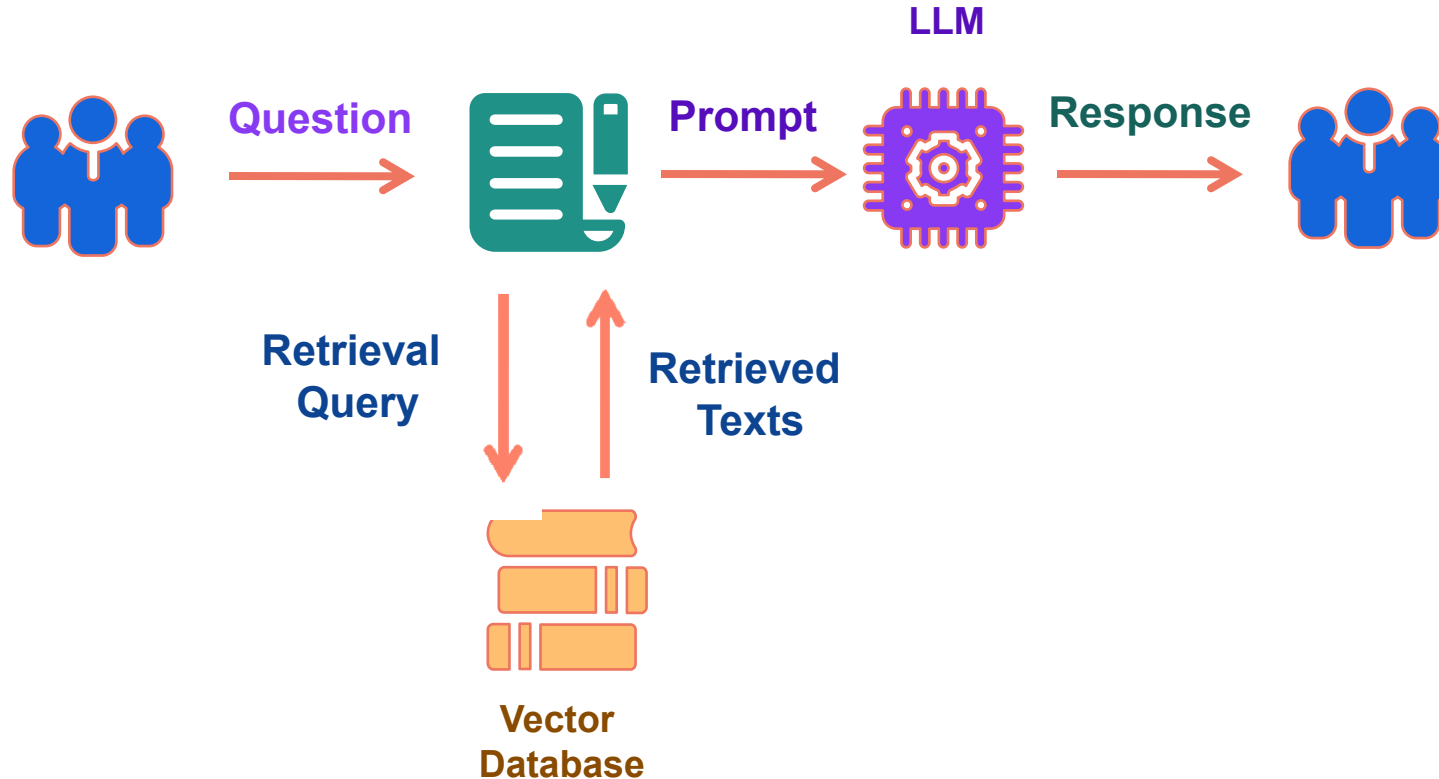
{0.78, 0.43,
0.34, 0.84}

{0.68, 0.24,
0.98, 0.01}

Store



Sahaayak – Retrieval Augmented Generation



Sahaayak – BARC Documents

[INST]

<<SYS>> You are a helpful, respectful, and honest assistant. ... If you don't know the answer to a question, please don't share false information. <</SYS>>

CONTEXT:

Magnesium -18's Unique Decay Process: ...

provides not only new academic insights but also practical solutions ...

Collaboration Identifies Rare Nuclear Decay in Long - Lived ...

Question: Describe decay process of Magnesium-18.

[/INST]

Sure! Based on the provided context, Magnesium-18 undergoes a unique multi-proton decay process, where it sequentially emits two proton pairs. ...

This process differs from traditional radioactive decay and highlights a complex phenomenon in the quantum world. ...

The study, published in the journal Nuclear Science and Techniques, provides ...

To summarize, Magnesium-18 decays through a chain of events, starting with the emission of two proton pairs, followed by the decay of Neon -16, ...

Sahaayak – BARC Documents

Q1. What is Neutron Transport?

Neutron Transport refers to the study of the movement of neutrons through a medium, such as a nuclear reactor core. It involves understanding how neutrons interact with the material they pass through, including absorption, scattering, and fission. The goal of neutron transport simulations is to predict the behaviour of the reactor and optimize its performance.

Q2. What is AHWR?

Based on the context text provided, AHWR stands for “Advanced Heavy Water Reactor.”

Q3. What is MSBR?

Based on the context provided, MSBR stands for Molten Salt Breeder Reactor.



Code Generation

Write Python function to find a factorial of an input number.

```
def factorial(n):  
    if n < 0:  
        raise ValueError("Factorial is not  
defined for negative numbers")  
    elif n == 0 or n == 1:  
        return 1  
    else:  
        return n * factorial(n-1)
```



Code Generation

Correct following Python code.

```
def factorial(n):  
    if n == 0 or n == 1:  
        return 1  
    else:  
        result = 1  
        for i in range(2, n + 1):  
            result *= i  
        return result
```

```
def factorial(n):  
    if n < 0:  
        raise ValueError("Factorial is not  
defined for negative numbers")  
    elif n == 0 or n == 1:  
        return 1  
    else:  
        return n * factorial(n-1)
```


Keyword Identification

List top ten keywords for following paragraph.

Image captioning models automatically generate image descriptions using semantics of the input image. ... In our current research work, we focus on designing and developing a fashion image captioning model for automating the generation of descriptive captions for fashion items. We call it the Fashion Vision-Language Model (FashionVLM) to capture the multi-modality nature of the model. We utilize a frozen large language model as a text decoder and a vision transformer as an image encoder, connecting these models with a comparatively smaller Querying Transformer. Fashion Captioning Dataset (FACAD) is one of the biggest datasets of fashion items. For fine-tuning on FACAD, we utilize BLIP-2 pretrain stage two and MS COCO fine-tuned models in three different stages. ... The OPT-6.7 based Stage Three FashionVLM achieves the best performance compared to the state-of-the-art for fashion captioning on FACAD, providing +4.281 points, + 39.015 points, +5.667 points, and + 3.519 points improvements for BLEU-4, CIDEr, ROUGE-L, and METEOR performance metrics respectively.

Here are the top ten keywords for the paragraph:

1. Fashion image captioning
2. Fashion Vision-Language Model (FashionVLM)
3. Large language model
4. Vision transformer
5. Querying Transformer
6. Fashion Captioning Dataset (FACAD)
7. BLIP-2
8. MS COCO
9. OPT-6.7
10. Fine-tuning

***Meta Llama 3.1 405B Instruct**

Pragya – Machine Learning Cluster

- 12 workstations
- Each workstation
 - Dual AMD EPYC Processors – 48 cores
 - 4 NVIDIA A100 GPUs
 - 6400GB NVMe SSD storage
 - 1TB Memory
- NVIDIA A100 GPU
 - 6912 CUDA cores
 - 80 GB memory

Falcon 180B On Pragya

- Falcon 180B Chat GPTQ
 - 180 Billion parameters
 - Instruction fine-tuned model
- Model compression
 - 180B parameters – 16 bit float – 360 GB memory
 - 180B parameters – 4 bit precision – ~94 GB memory
- Model parallelization
 - Divide model among multiple GPUs
 - ~24 GB – 4 A100 GPUs – ~94 GB / 4 GPUs

Conclusions

- Large Language Models
- Prompt Engineering
- In Context Learning
- Model Training
- Applications





Thank you

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Model Pre-training

- Self supervised learning
- Self annotations ($X - y$)
 - I love ice **cream**.
 - $X =$ I love ice
 - $y =$ **cream**.
- Learn language syntax
- Master language grammar
- Large amount of dataset
- Web scraping
- Vocabulary size
 - Number of tokens
 - 15.6 Trillion tokens

Instruction Fine Tuning

- Supervised learning
- Instructions and Responses
 - Question and Answer
 - Text and sentiment
 - English and Hindi sentences
- Generate accurate answers
- Generate appropriate answers

Reinforcement Learning with Human Feedback

- Reinforcement learning
- 3H – Helpful, Honest, Harmless

Code Generation

- Mistral AI
 - Mistral 7B and Mixtral 8X7B
- Meta
 - CodeLlama, CodeLlama-Python, CodeLlama-Instruct
- Phind
 - Phind-CodeLlama-34B, Phind-CodeLlama-34B-Python
- BigCode Project
 - StarCoder, StarCoder2

