



DDA5001 Final Project — Large Language Models

Part I - LLMs and Pre-training

Due: 23:59, November 16, 2025.

We guess that all of you, or at least almost all of you, are using GPT nowadays to do a lot of things (e.g., homework, coding, even for completing this project). In this project (three parts), we will study some basic working principles of these big AI models.

Contents

| | | |
|----------|---|----------|
| 1 | Introduction | 2 |
| 2 | Basics of Large Language Models (LLMs) | 2 |
| 2.1 | Prompts | 2 |
| 2.2 | Tokenization | 3 |
| 2.3 | LLM Modeling and Training Formulation | 4 |
| 2.3.1 | Language Modeling | 4 |
| 2.3.2 | Learning Problem Formulation of LLMs | 5 |
| 3 | Part I: Pre-train a GPT Model on Shakespeare Dataset | 5 |
| 3.1 | Dataset | 5 |
| 3.2 | Code structure | 6 |
| 3.3 | Task | 6 |
| 3.4 | Submission | 7 |
| 4 | Project Tutorials | 7 |

1 Introduction

Large Language Models (LLMs) are a transformative development in artificial intelligence and machine learning, with broad impact across applications such as text generation, translation, summarization, code synthesis, retrieval-augmented question answering, and tool use. Trained on large corpora of text (and increasingly multimodal data), these models can produce human-like outputs that are often coherent, informative, and contextually nuanced. Much of their capability arises from large-scale pre-training on next-token prediction using the Transformer architecture, hence the name “Generative Pre-trained Transformer” (GPT). During pre-training, models learn to predict the next token given previous context (see [Section 2.3](#)), implicitly acquiring linguistic structure, world knowledge, and useful reasoning patterns.

One of the most well-known LLMs is ChatGPT (with GPT-3.5, GPT-4, GPT-4o, GPT-5, o1, and o3 as its cores), developed by OpenAI, has demonstrated remarkable capabilities in understanding and generating text. It is widely utilized. There are also other representative models such as Claude by Anthropic, Gemini by Google, Llama by Meta, Qwen by Alibaba, to name a few. Nowadays, LLMs represent a significant advancement in the field of artificial intelligence, providing a convincing approach towards artificial general intelligence (AGI).

In this project, we aim to study several important elements of LLMs, including the modeling, training environment, simple pre-training, finetuning on math dataset, and reasoning model.

1. Part I (this part): Understand language modeling and install the training codes. Then, implement a simple (means small dataset) pre-training task for a simplified (means small size) yet very classic GPT model from scratch. In this part, you do not need to write codes. We will provide all the codes. Your task is to get familiar with LLM modeling and the training environment.
2. Part II (next part): Given a well pre-trained Qwen3 model (we will provide), perform fine-tuning on math datasets. You will need to write codes in this part. The aim is to see that fine-tuning can be important for improving downstream abilities such as math problem solving ability.
3. Part III (last part): Study reasoning models, that is, LLMs with strong mathematical reasoning ability. You will need to write codes in this part. We will see how sampling with different settings (as one method of test-time scaling) can improve the reasoning ability. We will use Qwen3 models in this part.

2 Basics of Large Language Models (LLMs)

2.1 Prompts

A prompt is the model’s steering wheel: a short specification that tells the model what to do, with what context, and in what style. Unlike a generic “input”, a well-crafted prompt guides behavior, small phrasing changes can shift tone, reasoning depth, or accuracy.

Typical ingredients:

- Task: What is needed (question, math, summarize, translate, classify, plan).
- Context: The evidence to use (passage, table, code, query).
- Constraints/style: Format, length, tone, schema.

Common forms (brief examples):

- Instruction style:

`Summarize the paragraph below in 2 bullets, each <12 words.`

- Few-shot (learn by example) style:

`Q: 2+2?`

`A: 4`

`Q: 3+5?`

`A:`

- Chain-of-thought (reason stepwise) style:

`Think step by step before giving the final answer.`

- Structured output style:

`Return JSON: {"verdict": "...", "evidence": ["...", "..."]}`.

- System + user (chat setup) style:

`[System] You are a precise, terse tutor.`

`[User] Explain dropout in one sentence.`

Why it matters: Prompts guide correctness, reduce hallucinations, and make LLMs useful without retraining. Even a simple sentence is a prompt, e.g.,

`Shenzhen is a great city.`

2.2 Tokenization

Before a model can process text, it must convert characters of the input prompt into discrete units called *tokens*. This conversion, *tokenization*, is handled by a *tokenizer*, which maps text to token IDs and back (via a vocabulary). Modern LLMs use subword tokenization (e.g., BPE, WordPiece, Unigram) to balance coverage and efficiency: Common words stay intact; rare words are split into meaningful pieces.

Why it matters:

- **Efficiency:** Fewer tokens per sentence means faster, cheaper inference.

- **Robustness:** Subwords handle misspellings, new words, and multilingual text.
- **Limits:** Context windows are measured in tokens, not characters.

Example (illustrative only; actual splits/IDs depend on the tokenizer):

Input: Shenzhen is a great city.

Subwords: Sh en zhen is a great city .

Token IDs: 50, 831, 46732, 318, 257, 1049, 1748, 13

Note: Different tokenizers (GPT-2 BPE, Llama SentencePiece, etc.) produce different splits and IDs.

Since in this part we will pre-train a GPT model, we use GPT-2’s tokenizer. It consists of 50257 tokens in total.

2.3 LLM Modeling and Training Formulation

2.3.1 Language Modeling

In almost all of the cases, LLM is an *auto-regressive* model (a.k.a. causal model), for predicting the next token. Given an input prompt \mathbf{x} , many language tasks are to predict what should be the next tokens \mathbf{y} , by choosing \mathbf{y} that has the largest conditional probability

$$\mathbb{P}[\mathbf{y}|\mathbf{x}]. \quad (1)$$

This is exactly the same as how we perform classification in logistic regression.

In LLMs, it models the conditional probability in (1) using an *auto-regressive Transformer*. Mathematically, it has the model

$$\mathbb{P}_{\mathbf{W}}[\mathbf{y}|\mathbf{x}] = \prod_{j=1}^m \mathbb{P}_{\mathbf{W}}[y_j|\mathbf{x}, \mathbf{y}_{1:j-1}]. \quad (2)$$

Here, “ $\mathbb{P}_{\mathbf{W}}$ ” is the transformer, and thus $\mathbf{W} \in \mathbb{R}^d$ encompasses all trainable parameters of the transformer, including the query, key, value, and output attention matrices, as well as the gate, up, and down projection matrices of each transformer layer. y_j is the j -th token in the output \mathbf{y} .

Hence, LLMs generate text in the following manner:

- (1) Receiving your input prompt \mathbf{x} (which may be a question or a story you would like the model to do the continuation) to the LLMs.
- (2) The LLMs will sample a y_1 from its vocabulary according to the distribution $\mathbb{P}_{\mathbf{W}}[y_1|\mathbf{x}]$.
- (3) Append the newly generated token y_1 to the input, giving $[x, y_1]$. Repeat the aforementioned steps by inputting $[x, y_1]$ into the model, until the maximum length / other stopping criterion is reached, which gives the generation \mathbf{y} .

2.3.2 Learning Problem Formulation of LLMs

The learning problem of LLMs is simply formulated from the maximum likelihood estimation (MLE) principle. That is, given a set of training data pairs $\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}$, the MLE learning problem of LLMs can be formulated as minimizing the negative log-likelihood of the generation probability:

$$\widehat{\mathbf{W}} \leftarrow \underset{\mathbf{W}}{\operatorname{argmin}} \mathcal{L}(\mathbf{W}) = \sum_{i \in \mathcal{D}} \sum_{j=1}^m -\log(\mathbb{P}_{\mathbf{W}}[y_{i,j} | \mathbf{x}_i, \mathbf{y}_{i,1:j-1}]). \quad (3)$$

Both pre-training and finetuning are using this learning problem formulation. The major difference between them lies in that they use different dataset \mathcal{D} .

3 Part I: Pre-train a GPT Model on Shakespeare Dataset

Part I is an **individual** project, where you are asked to pre-train a GPT model to generate text that mimics the style of Shakespeare. Because the task is very simple, we only need a small pre-training dataset. You do not need to write any code in this part, while you only need to learn the training environment and install it by yourself.

3.1 Dataset

We will use the Shakespeare dataset, which consists of 1,003,854 tokens (i.e., $n = 1,003,854$). We provide this dataset in project package. The following is a quick preview of the dataset:

First Citizen:

Before we proceed any further, hear me speak.

All:

Speak, speak.

First Citizen:

You are all resolved rather to die than to famish?

All:

Resolved. resolved.

First Citizen:

First, you know Caius Marcius is chief enemy to the people.

All:

We know't, we know't.

You can see that this is not normal English, but a style of special writing, i.e., Shakespeare.

3.2 Code structure

How to get our code and data: Our code and data for project Part I is available at <https://github.com/CUHKSZ-Course/DDA5001-25Fall>.

Our code is based on the NanoGPT¹. Here are the main files that you need to care about:

```
| README.md # project description and quick start
├─ p1/ # project part 1 directory
│   └─ src/ # main source code folder
│       ├── train.py # main file that implements the training logic
│       ├── model.py # definitions for the GPT model
│       ├── sample.py # code for model inference
│       └─ data/ # datasets and corresponding download scripts
```

If you do not have a powerful GPU (with at least 16GB RAM), you may have to use the free Tesla-P100 GPU offered by Kaggle platform. The following files are related to Kaggle setup:

```
| Kaggle_training.md # detailed instruction on using Kaggle GPU
├─ p1/ # project part 1 directory
│   ├── main.ipynb # notebook executed on Kaggle platform
│   ├── dataset-metadata-template.json # template for creating dataset-metadata.json
│   └─ kernel-metadata-template.json # template for creating kernel-metadata.json
```

3.3 Task

The objective of Part I is to setup the computational environment for running the experiment. To install the libraries, run

```
pip install torch numpy transformers datasets tiktoken wandb tqdm
```

Then, change `student_id` in `train.py` and `sample.py` to your own student id, e.g. 224040001. Run the following command to train a GPT model:

```
python train.py config/train_shakespeare_char.py
```

This will train a GPT model with the configuration specified in `config/train_shakespeare_char.py`. You should see the evolve of training loss and validation loss in the terminal output. Make sure that you have a GPU with enough memory when running the experiment, which can be either the Kaggle GPU or your own GPU. Do not attempt to use CPU since it is very slow. The checkpoint will be saved in the “out” directory automatically when the training is finished.

After you finishing pre-training, use the following command to generate text:

```
python sample.py --out_dir=out
```

This will automatically generate a Shakespeare-style text, without the need to provide a specific input prompt x .

¹<https://github.com/karpathy/nanoGPT>

3.4 Submission

1. A PDF report for Part I **up to one-page**. The page limit do not contain references pages and appendix. You can have two more pages for references and appendix. In this PDF, it should include
 - Plot the training loss and validation loss over 5000 steps in the same figure. Report the validation loss at iteration 5000.
 - Display the generated text for model trained at iteration 5000.
 - The difficulties (as well as how you solve them) and observations you had during completing project Part I.
2. Submit your checkpoint (i.e. the ckpt file) on Blackboard.
3. Since Part I is an **individual** work, everyone of you need to go through the process of installing this environment, running it, and submitting the report.

Note that there are **no** standard answers to the project. Different random seed may result in different performance, and different students may have different difficulties and observations. Once your results are reasonable, you can get the corresponding grades.

In terms of grades, Part I worth 30pts out of the 100pts of the whole project.

4 Project Tutorials

- We will have 3 tutorial (at 6:30pm - 7:30pm of Nov 4, Nov 18, Dec 2) to help you finish the project.
- These three tutorials will be **online** with zoom link: <https://cuhk-edu-cn.zoom.us/j/99410791830?pwd=bGR2NuHazCaaOF0PKhqYPf6ulb2bAq.1>. We will also provide **recordings** of these three tutorials.
- **Note:** We highly recommend that you attend (or go through the recording) every tutorial before completing each part. We will basically teach the main steps on how to complete the project.