GenAI Tutorial | 2025

LLMs From Scratch

Forough Shirin Abkenar

Contents

1 Overview **1**

2 LLMs Architecture **2**

3 Encoder-only Models **3**
3.1 Input Embedding . . . 3
3.2 Positional Encoding . . . 4
3.3 Encoder Layer . . . 5
3.3.1 Multi-Head Self-Attention Mechanism . . . 5
3.3.2 Add & Norm . . . 6
3.3.3 Feed-Forward Network . . . 6
3.4 Implementation . . . 7
3.4.1 Evaluation . . . 8

4 Decoder-only Models **9**
4.1 Input Embedding . . . 9
4.2 Positional Encoding . . . 11
4.3 Decoder Layer . . . 11
4.3.1 Multi-Head Self-Attention Mechanism . . . 11
4.3.2 Add & Norm . . . 12
4.3.3 Feed-Forward Network . . . 13
4.4 Implementation . . . 13
4.4.1 Evaluation . . . 15

5 LLM Fine-tuning **17**
5.1 Implementation . . . 17

6 PEFT **20**

7 RLHF **21**

8 RAG **22**

9 Agentic AI **23**

10 References **24**

List of Figures

2.1 Architecture of an LLM 2

3.1 Encoder-only mode architecture 3
3.2 Architecture of an attention head 5

4.1 Decoder-only mode architecture 9
4.2 Architecture of an attention head 12

5.1 Overall workflow of fine-tuning. 17

List of Tables

3.1 Performance evaluation of tinyBERT 8

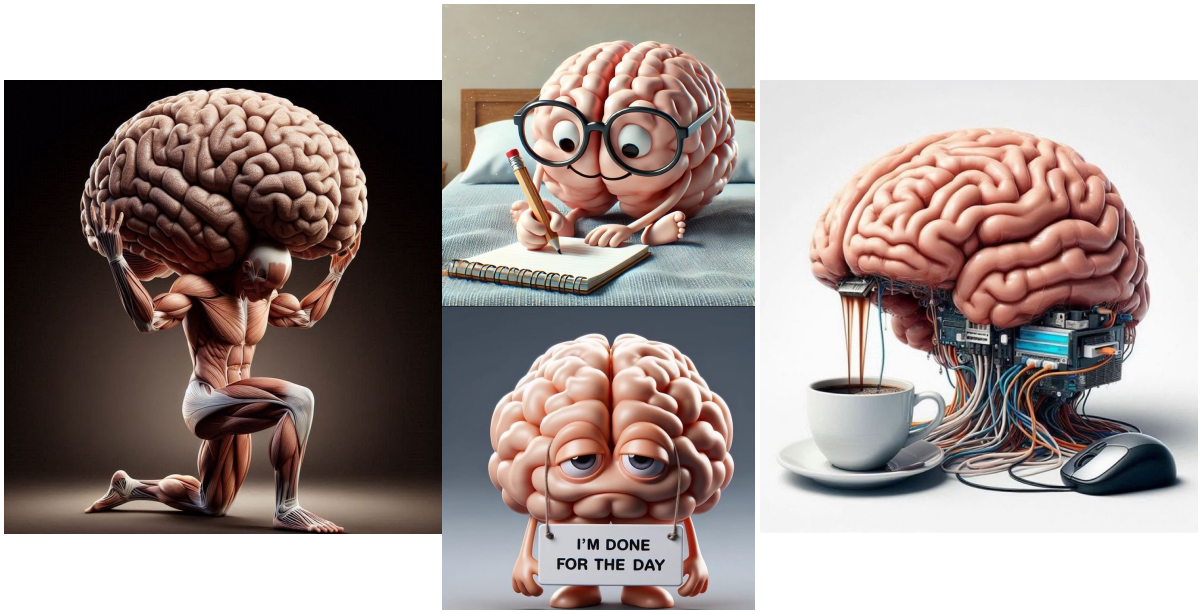
4.1 Performance evaluation of TinyGPT 16

5.1 Performance evaluation of the fine-tuned model 19

Overview

The current document studies fundamental topics related to generative artificial intelligence (AI) and large language models (LLMs) [1], such as model architectures and optimizations, fine-tuning, and agentic systems, and the corresponding codes are implemented in Python and PyTorch. For implementation purposes, we also use defined tokenizers, models, and agents in HuggingFace [2] and LangChain [3]. It is worth noting

that the cliparts used in this document were downloaded from Pinterest [4].



LLMs Architecture

Transformers form the foundation of large language model (LLM) architectures. The original LLM architecture consists of two main components, named as an encoder and a decoder (see Fig. 2.1) [1]. Models that follow this design are referred to as *encoder-decoder models*. In these models, the encoder embeds the input, and the resulting representation is passed to the decoder for further processing. Building on the capabilities of these two components, two additional LLM architectures were later introduced, namely *encoder-only* and *decoder-only* models. The following two sections review these architectures in detail. It is worth mentioning that the encoder-decoder architecture is beyond the scope of the current document.

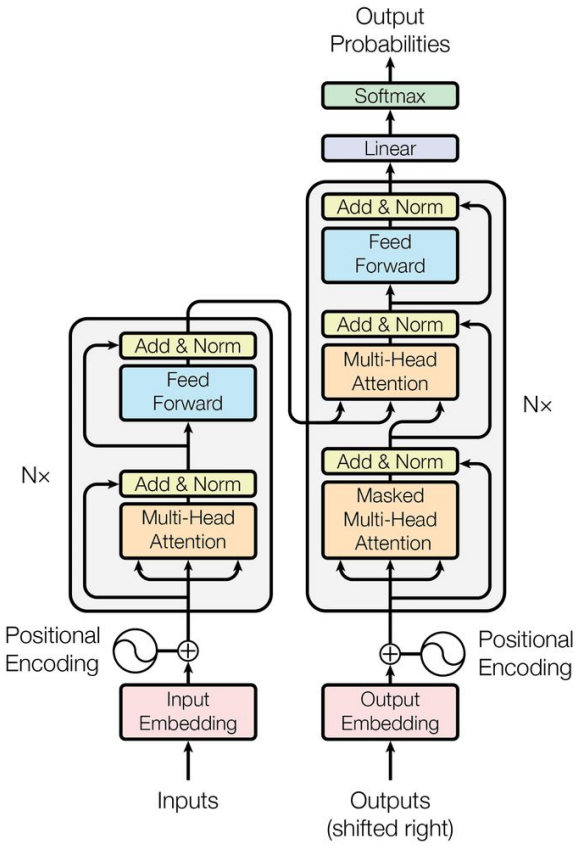


Figure 2.1: Architecture of an LLM including an encoder and a decoder [1].

Encoder-only Models

The encoder-only models in LLMs owns the LLM architecture with only the encoder transformer (see Fig. 3.1). The encoder in the LLM architecture is responsible for receiving the input data (prompts) and embedding (encoding) them into meaningful output (vector representation). Encoder-only models exploit bidirectional processing of data whereby the input tokens are processed using information from both left and right to understand the token's context.

Bidirectional encoder representations from transformers (BERT) [5] and robustly optimized BERT pretraining approach (RoBERTa) [6] models are examples of encoder-only models that are applicable for text classification, sentiment analysis, named entity recognition (NER), and etc.

As seen in Fig. 3.1, the inputs in the encoder-only model are passed through sequential components, i.e., input embedding, positional encoding, and encoder layer (shown as Nx in the figure). In the rest of the current chapter, we review each layer and the corresponding mechanisms.

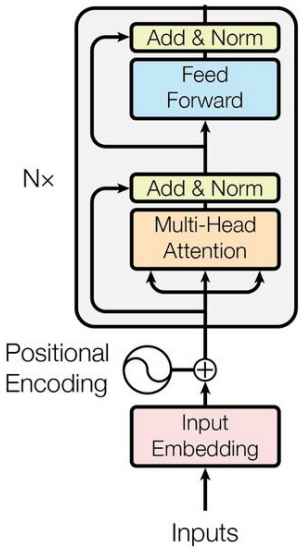


Figure 3.1: Encoder-only mode architecture [1].

3.1 Input Embedding

In encoder-only models, the inputs are textual data, represented as sequences of text units such as words, subwords, or characters. However, the encoder block processes numerical representations rather than raw text. To bridge this gap, an *input embedding* layer converts textual inputs into numerical IDs. This process relies on a predefined *vocabulary* in which each text unit, commonly referred to as a *token*, is mapped to a unique identifier, namely token ID. Notably, each token ID is a vector of numbers with a shape of pr-defined embedding dimension. Consequently, the input text undergoes *tokenization*, where it is divided into tokens, and then each token is mapped to the corresponding token ID.

For instance, in a Python programming, we define the input as

```
# Input
text ="""
Jalāl al-Dīn Muḥammad Rūmī, or simply Rumi, was a 13th-century poet, Hanafi
faqih, Maturidi theologian, and Sufi mystic born during the Khwarazmian Empire.
"""
```

In the next step, we need to define the tokens unit. Considering the word unit as the tokens, we have

```
# Data preparation for the vocabulary

# remove newlines
text = text.replace('\n', ' ')

# convert text to characters
words = text.split()
print(f"Words: {words}")

# size of vocabulary
vocab = list(set(words))
vocab_size = len(vocab)
```

```
Words: ['Jalāl', 'al-Dīn', 'Muḥammad', 'Rūmī,', 'or', 'simply', 'Rumi,', 'was', 'a', '13th-century', 'poet,', 'Hanafi', 'faqih,', 'Matur
idi', 'theologian,', 'and', 'Sufi', 'mystic', 'born', 'during', 'the', 'Khwarazmian', 'Empire.']
```

Finally, the tokens are converted into token IDs. To achieve this, the vocabulary (stoi in the code) is defined, and the *encode* function is applied to the input text.

```
# Encoding

# string to integer
stoi = {c: i for i, c in enumerate(vocab)}
results = []
for k, v in stoi.items():
    results.append(f"{k}: {v}")
print(results)

# define the encoder
encode = lambda s: torch.tensor([stoi[c] for c in s.split()], dtype=torch.long)

encoded_text = encode(text)
print(f"\nEncoded text: {encoded_text}")
```

```
['poet,: 0', 'al-Dīn: 1', 'faqih,: 2', 'and: 3', 'Muḥammad: 4', 'born: 5', 'Hanafi: 6', 'was: 7', 'Rūmī,: 8', 'Rumi,: 9', 'or: 10', 'sim
ply: 11', 'a: 12', 'Khwarazmian: 13', 'Sufi: 14', 'mystic: 15', 'theologian,: 16', 'Maturidi: 17', 'the: 18', 'Jalāl: 19', '13th-centur
y: 20', 'Empire.: 21', 'during: 22']

Encoded text: tensor([19,  1,  4,  8, 10, 11,  9,  7, 12, 20,  0,  6,  2, 17, 16,  3, 14, 15,
         5, 22, 18, 13, 21])
```

3.2 Positional Encoding

Positional encoding is a mechanism whereby the information about the position of a token is injected to the input data. Hence, the model can learn the meaning and importance of the corresponding token w.r.t. its position in the input (subject, object, verb, adjective, etc.). The traditional positional encoding is calculated using Eq. 3.1, where pos, i, and d_{model} are position, the index for the dimension, and the embedding dimension [1].

$$\begin{aligned} PE_{(pos,i)} &= \sin\left(pos/10000^{2i/d_{\text{model}}}\right) \\ PE_{(pos,2i+1)} &= \cos\left(pos/10000^{2i/d_{\text{model}}}\right) \end{aligned} \tag{3.1}$$

It is worth noting that positional encoding can also be learned during the training of the encoder. For example, in the following code snippet, the positional encoding is implemented as a dedicated layer within the model. During the forward pass, the positional information is integrated into the input representations by adding it to the token embeddings.

```python
class TinyBERT(nn.Module):
    def __init__(self, vocab_size, block_size, n_embed=128, n_head=4, n_layer=4, dropout=0.1):
        super(TinyBERT, self).__init__()
        self.token_embed = nn.Embedding(vocab_size, n_embed)
        self.pos_embed = nn.Embedding(block_size, n_embed)
        self.blocks = nn.Sequential(
            *[Block(n_embed, n_head, dropout) for _ in range(n_layer)]
        )
        self.ln_f = nn.LayerNorm(n_embed)
        self.mlm_head = nn.Linear(n_embed, vocab_size)

    def forward(self, idx, labels=None):
        B, T = idx.shape
        token = self.token_embed(idx)
        pos = self.pos_embed(torch.arange(T, device=idx.device))
        x = token + pos
        x = self.blocks(x)
        x = self.ln_f(x)
        logits = self.mlm_head(x)
        loss = None
        if labels is not None:
            loss = F.cross_entropy(logits.view(-1, logits.size(-1)), labels.view(-1), ignore_index=-100)

        return logits, loss
```

3.3 Encoder Layer

The encoder layer (shown Nx in Fig. 3.1) comprises two sub-layers. The first sub-layer implements the multi-head self-attention mechanism, and the second sub-layer is a fully-connected feed-forward neural network. Each sub-layer has a residual connection around itself, and also is succeeded by a normalization layer [1].

3.3.1 Multi-Head Self-Attention Mechanism

The self-attention mechanism is a core component of transformers, enabling the model to learn and capture the relationships between tokens within a sequence. This mechanism is implemented within the attention heads of the transformer architecture [1].

To model the relationships between tokens, the input is first projected into three distinct representations: the *query* (Q), *key* (K), and *value* (V) vectors. Figure 3.2 illustrates the architecture of an attention head within the model. When an embedded and positionally encoded input passes through the attention head, it undergoes the following five processing steps [1]:

- **Step 1:** query (Q), key (K), and value (V) components are passed through linear layers in the attention head model so that these components are learned.
- **Step 2:** the alignment scores are calculated through multiplication of matrices query and key.
- **Step 3:** the alignment scores are scaled by $1/d_k$, where d_k is the dimension of the query (or the key) matrix.
- **Step 4:** *softmax* operation is applied to the scaled scores to obtain the attention weights.
- **Step 5:** the attention weights are multiplied with the value matrix.

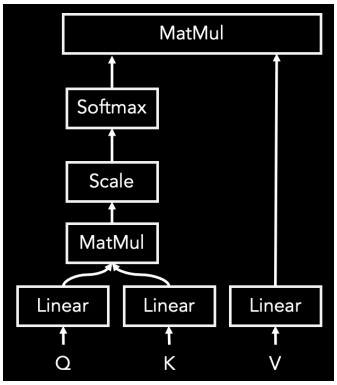
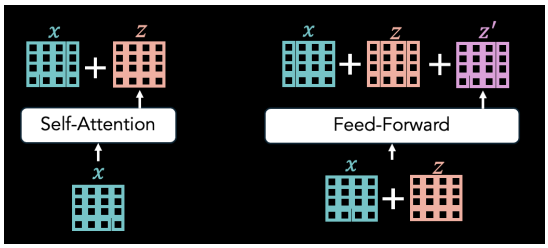


Figure 3.2: Architecture of an attention head [1].

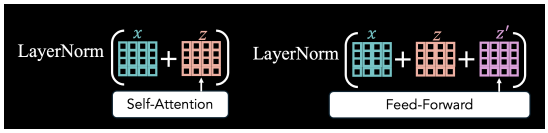
The multi-head self-attention mechanism consists of multiple parallel attention heads, each learning distinct representation subspaces. The outputs from all attention heads are concatenated and then projected through a linear layer to produce the final combined representation [1].

3.3.2 Add & Norm

Residual Connections (Add): Preserving information from earlier layers helps mitigate the vanishing gradient problem. In transformer encoders, this is achieved through *residual connections*, where the original input of a layer is added to its output. This mechanism enables the network to retain essential information across layers and facilitates more effective gradient flow during training [1].



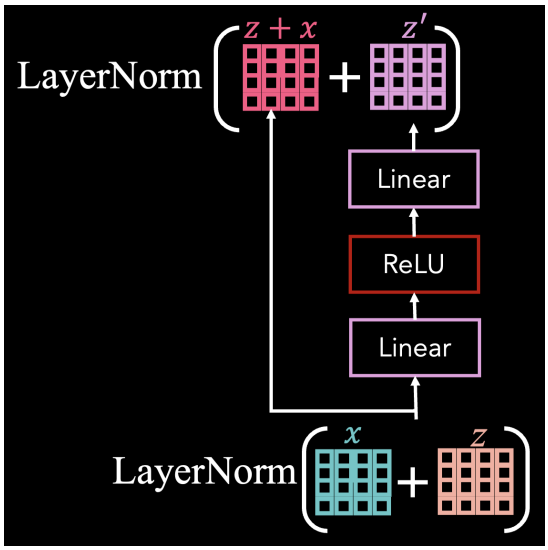
Layer Normalization (Norm): During training, the model may experience *internal covariate shift*, where the distribution of activations changes across layers, potentially leading to vanishing or exploding gradients. To address this challenge, *layer normalization* is applied to the outputs of deeper layers that in result, stabilizes training by reducing distributional shifts and ensures more consistent gradient flow [1].



3.3.3 Feed-Forward Network

The feed-forward sub-layer introduces non-linearities into the encoder, thereby enhancing the model's capacity to capture complex patterns and non-linear relationships within sequential data. The feed-forward network consists of two linear transformations separated by an activation function, typically the rectified linear unit (ReLU) or the Gaussian error linear unit (GELU) [1].

The ReLU activation applies $\max(0, x)$ to each input x, effectively setting all negative values to zero. Although computationally efficient, ReLU suffers from the *dying ReLU* problem, where neurons can become permanently inactive during training and consistently output zero due to negative weighted inputs. In contrast, GELU is a smoother activation function that maps a value to $x \times \Phi(x)$, where $\Phi(x)$ denotes the cumulative distribution function (CDF) of the standard normal distribution. This smooth approximation allows GELU to retain small negative values and has been shown to improve performance in transformer-based architectures [1].



3.4 Implementation

In this section, we use a small input text to develop a minimal encoder-only model, called **TinyBert**. The goal is to gain familiarity with the operation of encoder-only models. The overall network architecture is shown below, and the complete implementation script is available on GitHub.

```python
class TinyBERT(nn.Module):
    def __init__(self, vocab_size, block_size, n_embed=128, n_head=4, n_layer=4, dropout=0.1):
        super(TinyBERT, self).__init__()
        self.token_embed = nn.Embedding(vocab_size, n_embed)
        self.pos_embed = nn.Embedding(block_size, n_embed)
        self.blocks = nn.Sequential(
            *[Block(n_embed, n_head, dropout) for _ in range(n_layer)]
        )
        self.ln_f = nn.LayerNorm(n_embed)
        self.mlm_head = nn.Linear(n_embed, vocab_size)

    def forward(self, idx, labels=None):
        B, T = idx.shape
        token = self.token_embed(idx)
        pos = self.pos_embed(torch.arange(T, device=idx.device))
        x = token + pos
        x = self.blocks(x)
        x = self.ln_f(x)
        logits = self.mlm_head(x)
        loss = None
        if labels is not None:
            loss = F.cross_entropy(logits.view(-1, logits.size(-1)), labels.view(-1), ignore_index=-100)

        return logits, loss
```

As defined in the ___*init*___ function, the model network includes the following layers:

- self.token_embed: it creates an embedding layer that converts token indices (integers) into dense vector representations (embeddings).
- self.pos_embed: this layer create the positional encoding of the input tokens.
- self.blocks: it includes encoder blocks (layers), each with a multi-head self-attention head, a feed-forward network, and the corresponding add & norm components.
- self.ln_f: this layer defines the final layer normalization applied to the transformer's output before passing it into the language modeling head.
- self.mlm_head: it defines the masked language model (MLM) head, i.e., the final layer that maps the hidden representations produced by the transformer into predicted token probabilities.

When an input passes through the *forward* function, it is first converted into token embeddings. Positional embeddings are then added to incorporate information about token order. The resulting representations are sequentially passed through all the transformer blocks defined in the model. The output of the final block is normalized using the last layer normalization and then fed into the language modeling head. At this stage, each token is represented by a hidden vector of size equal to the embedding dimension, and the final layer predicts the probability distribution over the vocabulary for the next token.

```python
class Head(nn.Module):
    def __init__(self, n_embed, head_size, dropout):
        super(Head, self).__init__()
        self.key = nn.Linear(n_embed, head_size, bias=False)
        self.query = nn.Linear(n_embed, head_size, bias=False)
        self.value = nn.Linear(n_embed, head_size, bias=False)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        B, T, C = x.shape
        k, q, v = self.key(x), self.query(x), self.value(x)
        att = (q @ k.transpose(-2, -1)) / math.sqrt(k.size(-1))
        att = F.softmax(att, dim=-1)
        att = self.dropout(att)
        out = att @ v

        return out
```

```python
class MultiHead(nn.Module):
    def __init__(self, n_embed, n_head, dropout):
        super(MultiHead, self).__init__()
        head_size = n_embed // n_head
        self.heads = nn.ModuleList(
            [Head(n_embed, head_size, dropout) for _ in range(n_head)]
        )
        self.proj = nn.Linear(n_embed, n_embed)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        out = torch.cat([h(x) for h in self.heads], dim=-1)
        proj = self.proj(out)
        return self.dropout(proj)
```

```python
class FeedForward(nn.Module):
    def __init__(self, n_embed, dropout):
        super(FeedForward, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(n_embed, 4*n_embed),
            nn.GELU(),
            nn.Linear(4*n_embed, n_embed),
            nn.Dropout(dropout)
        )

    def forward(self, x):
        return self.net(x)
```

```python
class Block(nn.Module):
    def __init__(self, n_embed, n_head, dropout):
        super(Block, self).__init__()
        self.mh = MultiHead(n_embed, n_head, dropout)
        self.ff = FeedForward(n_embed, dropout)
        self.ln1 = nn.LayerNorm(n_embed)
        self.ln2 = nn.LayerNorm(n_embed)

    def forward(self, x):
        x_p = self.ln1(x)
        x = x + self.mh(x_p)
        x_p = self.ln2(x)
        x = x + self.ff(x_p)

        return x
```

During training, the model compares these predicted logits with the true token IDs using cross-entropy loss, and updates its weights through backpropagation to minimize this loss.

```
num_epochs = 1000
for epoch in range(num_epochs):
    x_batch, y_batch = get_batch(mask_token_id, vocab_size, batch_size=BATCH_SIZE, block_size=BLOCK_SIZE)
    logits, loss = model(x_batch, y_batch)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    mask = y_batch != -100
    preds = torch.argmax(logits, dim=-1)
    correct = (preds[mask] == y_batch[mask]).sum().item()
    acc = correct / mask.sum().item()

    if (epoch + 1) % 100 == 0:
        print(f"Epoch {epoch + 1}/{num_epochs}, Loss: {loss.item(): .4f}, Accuracy: {acc * 100: .2f}")
```

```
Epoch 100/1000, Loss:  4.8240, Accuracy:  5.88
Epoch 200/1000, Loss:  3.9187, Accuracy:  16.67
Epoch 300/1000, Loss:  3.5331, Accuracy:  30.43
Epoch 400/1000, Loss:  2.6440, Accuracy:  46.81
Epoch 500/1000, Loss:  2.0034, Accuracy:  70.00
Epoch 600/1000, Loss:  1.5215, Accuracy:  65.96
Epoch 700/1000, Loss:  1.3033, Accuracy:  74.00
Epoch 800/1000, Loss:  1.0863, Accuracy:  86.67
Epoch 900/1000, Loss:  0.6710, Accuracy:  91.89
Epoch 1000/1000, Loss:  0.6087, Accuracy:  95.83
```

Since the primary objective of the designed TinyBert model is to predict masked tokens in the input text, the *get_batch* function used during training incorporates a *mask_token* function based on the MLM strategy. This function applies an 80/10/10 masking rule: 80% of tokens are replaced with a predefined mask token (e.g., "[MASK]"), 10% are substituted with random tokens from the vocabulary, and the remaining 10% are left unchanged.

```
data = encode(text)
def get_batch(mask_token_id, vocabsize, batch_size=32, block_size=8):
    ix = torch.randint(0, len(data) - block_size - 1, (batch_size,))
    x = torch.stack([data[i: i+block_size] for i in ix])            # (batch_size, block_size)
    y = torch.stack([data[i+1: i+1+block_size] for i in ix])        # (batch_size, block_size)
    x, y = mask_tokens(x.clone(), vocabsize, mask_token_id)

    return x.to(DEVICE), y.to(DEVICE)
```

3.4.1 Evaluation

For evaluation, we select a portion of the text, mask certain words, and assess the model's performance in predicting these masked tokens. Accordingly, we compute the cross-entropy loss, perplexity, and accuracy on the masked words: (1) cross-entropy loss measures the difference between the predicted probability distribution of a model and the true distribution of the target data; lower values indicates better predictions and less uncertainty. (2) perplexity measures the model's uncertainty; lower perplexity implies that the model assigns higher probability to the actual next word in the sequence, resulting a more confident and accurate model. (3) accuracy measures how well the model predicts the masked tokens, with higher values indicating more correct predictions. Table 3.1 indicates the performance of TinyBert w.r.t. the aforementioned evaluation metrics.

Table 3.1: Performance evaluation of tinyBERT

Cross-Entropy Loss	**Perplexity**	**Accuracy (%)**
0.2245	1.25	100

Decoder-only Models

Decoder-only models in LLMs consist solely of the transformer decoder component of the overall architecture (see Fig. 4.1). The decoder receives input data (prompts) and generates coherent and context-aware output. Unlike encoder-only models, which leverage bidirectional context, decoder-only models are **autoregressive** whereby they predict the next token based on the previously generated tokens. Therefore, these models are particularly well-suited for text generation tasks.

Generative pre-trained transformer (GPT) family (e.g., GPT-2, GPT-3, and ChatGPT) [7], pathways language model (PaLM) [8], and large language model Meta AI (LlaMA) [9] models are examples of decoder-only models, commonly used for text generation tasks such as creative writing and conversational agents.

As shown in Fig. 4.1, similar to encoder-only models, the inputs in a decoder-only model are processed through a series of sequential components, including input embedding, positional encoding, and decoder blocks/layers (denoted as Nx in the figure). In the remainder of this chapter, we review each layer and its underlying mechanisms in detail.

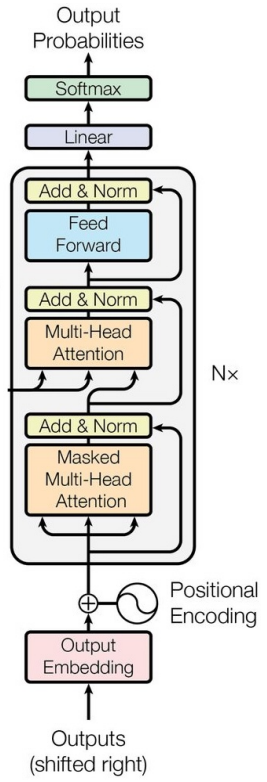


Figure 4.1: Decoder-only mode architecture [1].

4.1 Input Embedding

In decoder-only models, the inputs are textual data, represented as sequences of text units such as words, subwords, or characters. However, the decoder block processes numerical representations rather than raw text. To bridge this gap, an *input embedding* layer converts textual inputs into numerical IDs. This process relies on a predefined *vocabulary* in which each text unit, commonly referred to as a *token*, is mapped to a unique identifier, namely token ID. Notably, each token ID is a vector of numbers with a shape of pr-defined embedding dimension. Consequently, the input text undergoes *tokenization*, where it is divided into tokens, and then each token is mapped to the corresponding token ID.
For instance, in a Python programming, we define the input as

```
text = """
Jalāl al-Dīn Muḥammad Rūmī, or simply Rumi, was a 13th-century poet, Hanafi
faqih, Maturidi theologian, and Sufi mystic born during the Khwarazmian Empire.
Rumi's works are written in his mother tongue, Persian. He occasionally used the
Arabic language and single Turkish and Greek words in his verse."""
```

In the next step, we need to define the tokens unit. Considering the character unit as the tokens, we have

```
# Data preparation for the vocabulary

# convert text to characters
chars = list(set(text))
```

Finally, the tokens are converted into token IDs. To achieve this, the vocabulary (stoi in the code) is defined, and the *encode* function is applied to the input text.

```
# Encoding

# string to integer
stoi = {c: i for i, c in enumerate(chars)}
results = []
for k, v in stoi.items():
    results.append(f"{k}: {v}")
print(results)

# encode
encode = lambda s: torch.tensor([stoi[c] for c in s], dtype=torch.long)

encoded_text = encode(text)
print(f"\nEncoded text: {encoded_text}")
```

```
['z: 0', 'd: 1', 'ī: 2', '\n: 3', 'u: 4', 'q: 5', ',: 6', 'k: 7', 'o: 8', "': 9", 'ḥ: 10', 'h: 11', 'P: 12', 'm: 13', ' : 14', 'ā: 15',
'b: 16', 'l: 17', 'i: 18', 'M: 19', 'R: 20', 'n: 21', 'E: 22', 's: 23', 'a: 24', '–: 25', 'w: 26', '1: 27', 'p: 28', '.: 29', 'f: 30',
'ū: 31', 'K: 32', 't: 33', 'y: 34', 'A: 35', 'H: 36', 'T: 37', 'e: 38', 'r: 39', 'v: 40', 'c: 41', 'G: 42', '3: 43', 'J: 44', 'D: 45',
'g: 46', 'S: 47']

Encoded text: tensor([ 3, 44, 24, 17, 15, 17, 14, 24, 17, 25, 45,  2, 21, 14, 19,  4, 10, 24,
        13, 13, 24,  1, 14, 20, 31, 13,  2,  6, 14,  8, 39, 14, 23, 18, 13, 28,
        17, 34, 14, 20,  4, 13, 18,  6, 14, 26, 24, 23, 14, 24, 14, 27, 43, 33,
        11, 25, 41, 38, 21, 33,  4, 39, 34, 14, 28,  8, 38, 33,  6, 14, 36, 24,
        21, 24, 30, 18, 14,  3, 30, 24,  5, 18, 11,  6, 14, 19, 24, 33,  4, 39,
        18,  1, 18, 14, 33, 11, 38,  8, 17,  8, 46, 18, 24, 21,  6, 14, 24, 21,
         1, 14, 47,  4, 30, 18, 14, 13, 34, 23, 33, 18, 41, 14, 16,  8, 39, 21,
        14,  1,  4, 39, 18, 21, 46, 14, 33, 11, 38, 14, 32, 11, 26, 24, 39, 24,
         0, 13, 18, 24, 21, 14, 22, 13, 28, 18, 39, 38, 29, 14,  3, 20,  4, 13,
        18,  9, 23, 14, 26,  8, 39,  7, 23, 14, 24, 39, 38, 14, 26, 39, 18, 33,
        33, 38, 21, 14, 18, 21, 14, 11, 18, 23, 14, 13,  8, 33, 11, 38, 39, 14,
        33,  8, 21, 46,  4, 38,  6, 14, 12, 38, 39, 23, 18, 24, 21, 29, 14, 36,
        38, 14,  8, 41, 41, 24, 23, 18,  8, 21, 24, 17, 17, 34, 14,  4, 23, 38,
         1, 14, 33, 11, 38, 14,  3, 35, 39, 24, 16, 18, 41, 14, 17, 24, 21, 46,
         4, 24, 46, 38, 14, 24, 21,  1, 14, 23, 18, 21, 46, 17, 38, 14, 37,  4,
        39,  7, 18, 23, 11, 14, 24, 21,  1, 14, 42, 39, 38, 38,  7, 14, 26,  8,
        39,  1, 23, 14, 18, 21, 14, 11, 18, 23, 14, 40, 38, 39, 23, 38, 29])
```

Moreover, a *decode* function is defined to convert tokens IDs to tokens. To this end, we defined the corresponding dictionary (itos in the code), and the *decode* function is applied to the encoded text.

```
# Decoding

# integer to string
itos = {i: c for c, i in stoi.items()}

# decode
decode = lambda t: ''.join(itos[int(i)] for i in t)

decoded_text = decode(encoded_text)
print(f"Decoded IDs: {decoded_text}")
```

```
Decoded IDs:
Jalāl al-Dīn Muḥammad Rūmī, or simply Rumi, was a 13th-century poet, Hanafi
faqih, Maturidi theologian, and Sufi mystic born during the Khwarazmian Empire.
Rumi's works are written in his mother tongue, Persian. He occasionally used the
Arabic language and single Turkish and Greek words in his verse.
```

4.2 Positional Encoding

Positional encoding is a mechanism whereby the information about the position of a token is injected to the input data. Hence, the model can learn the meaning and importance of the corresponding token w.r.t. its position in the input (subject, object, verb, adjective, etc.). The traditional positional encoding is calculated using Eq. 4.1, where pos, i, and d_{model} are position, the index for the dimension, and the embedding dimension [1].

$$\begin{aligned} PE_{(pos,i)} &= \sin\left(pos/10000^{2i/d_{\text{model}}}\right) \\ PE_{(pos,2i+1)} &= \cos\left(pos/10000^{2i/d_{\text{model}}}\right) \end{aligned} \tag{4.1}$$

It is worth noting that positional encoding can also be learned during the training of the encoder. For example, in the following code snippet, the positional encoding is implemented as a dedicated layer within the model. During the forward pass, the positional information is integrated into the input representations by adding it to the token embeddings.

```python
class TinyGPT(nn.Module):
    def __init__(self, vocab_size, block_size, n_embed=128, n_head=4, n_layer=4, dropout=0.1):
        super(TinyGPT, self).__init__()
        self.token_embed = nn.Embedding(vocab_size, n_embed)
        self.pos_embed = nn.Embedding(block_size, n_embed)
        self.blocks = nn.Sequential(
            *[Block(n_embed, n_head, block_size, dropout) for _ in range(n_layer)]
        )
        self.ln_f = nn.LayerNorm(n_embed)
        self.lm_head = nn.Linear(n_embed, vocab_size)

    def forward(self, idx, targets=None):
        B, T = idx.shape
        token = self.token_embed(idx)
        pos = self.pos_embed(torch.arange(T, device=idx.device))
        x = token + pos
        x = self.blocks(x)
        x = self.ln_f(x)
        logits = self.lm_head(x)
        loss = None
        if targets is not None:
            loss = F.cross_entropy(logits.view(-1, logits.size(-1)), targets.view(-1))

        return logits, loss
```

4.3 Decoder Layer

The decoder layer (shown as Nx in Fig. 4.1) consists of three sub-layers: (1) a multi-head self-attention mechanism applied to the decoder's inputs, (2) a multi-head cross-attention mechanism over the encoder's outputs, and (3) a fully connected feed-forward network. Each sub-layer includes a residual connection and is followed by a normalization layer [1].

4.3.1 Multi-Head Self-Attention Mechanism

The self-attention mechanism is a core component of transformers, enabling the model to learn and capture the relationships between tokens within a sequence. This mechanism is implemented within the attention heads of the transformer architecture [1].

To model the relationships between tokens, the input is first projected into three distinct representations: the *query* (Q), *key* (K), and *value* (V) vectors. Figure 4.2 illustrates the architecture of an attention head within the model. When an embedded and positionally encoded input passes through the attention head, it undergoes the following six processing steps [1]:

- **Step 1:** query (Q), key (K), and value (V) components are passed through linear layers in the attention head model so that these components are learned.
- **Step 2:** the alignment scores are calculated through multiplication of matrices query and key.
- **Step 3:** the alignment scores are scaled by $1/d_k$, where d_k is the dimension of the query (or the key) matrix.
- **Step 4:** a causal masking function is applied to prevent the model from attending to future tokens.
- **Step 5:** *softmax* operation is applied to the scaled scores to obtain the attention weights.
- **Step 6:** the attention weights are multiplied with the value matrix.

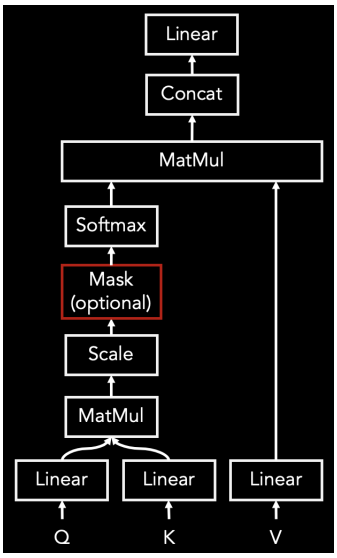
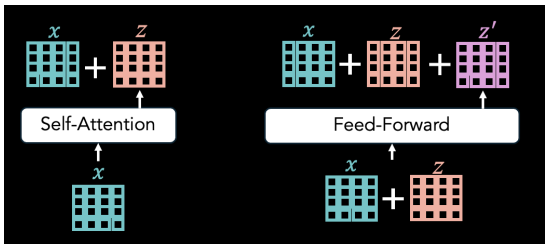


Figure 4.2: Architecture of an attention head [1].

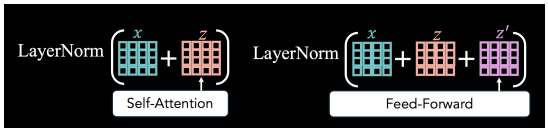
The multi-head self-attention mechanism consists of multiple parallel attention heads, each learning distinct representation subspaces. The outputs from all attention heads are concatenated and then projected through a linear layer to produce the final combined representation [1].

4.3.2 Add & Norm

Residual Connections (Add): Preserving information from earlier layers helps mitigate the vanishing gradient problem. In transformer encoders, this is achieved through *residual connections*, where the original input of a layer is added to its output. This mechanism enables the network to retain essential information across layers and facilitates more effective gradient flow during training [1].



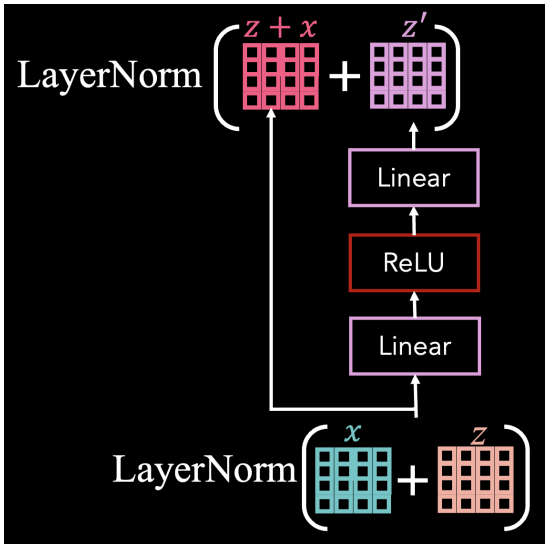
Layer Normalization (Norm): During training, the model may experience *internal covariate shift*, where the distribution of activations changes across layers, potentially leading to vanishing or exploding gradients. To address this challenge, *layer normalization* is applied to the outputs of deeper layers that in result, stabilizes training by reducing distributional shifts and ensures more consistent gradient flow [1].



4.3.3 Feed-Forward Network

The feed-forward sub-layer introduces non-linearities into the encoder, thereby enhancing the model's capacity to capture complex patterns and non-linear relationships within sequential data. The feed-forward network consists of two linear transformations separated by an activation function, typically the Rectified Linear Unit (ReLU) or the Gaussian Error Linear Unit (GELU) [1].

The ReLU activation applies $\max(0, x)$ to each input x, effectively setting all negative values to zero. Although computationally efficient, ReLU suffers from the *dying ReLU* problem, where neurons can become permanently inactive during training and consistently output zero due to negative weighted inputs. In contrast, GELU is a smoother activation function that maps a value to $x \times \Phi(x)$, where $\Phi(x)$ denotes the cumulative distribution function (CDF) of the standard normal distribution. This smooth approximation allows GELU to retain small negative values and has been shown to improve performance in transformer-based architectures [1].



4.4 Implementation

In this section, we use a small input text to develop a minimal decoder-only model, called **TinyGPT**. The goal is to gain familiarity with the operation of decoder-only models. The overall network architecture is shown below, and the complete implementation script is available on GitHub.

```
class TinyGPT(nn.Module):
    def __init__(self, vocab_size, block_size, n_embed=128, n_head=4, n_layer=4, dropout=0.1):
        super(TinyGPT, self).__init__()
        self.token_embed = nn.Embedding(vocab_size, n_embed)
        self.pos_embed = nn.Embedding(block_size, n_embed)
        self.blocks = nn.Sequential(
            *[Block(n_embed, n_head, block_size, dropout) for _ in range(n_layer)]
        )
        self.ln_f = nn.LayerNorm(n_embed)
        self.lm_head = nn.Linear(n_embed, vocab_size)

    def forward(self, idx, targets=None):
        B, T = idx.shape
        token = self.token_embed(idx)
        pos = self.pos_embed(torch.arange(T, device=idx.device))
        x = token + pos
        x = self.blocks(x)
        x = self.ln_f(x)
        logits = self.lm_head(x)
        loss = None
        if targets is not None:
            loss = F.cross_entropy(logits.view(-1, logits.size(-1)), targets.view(-1))

        return logits, loss
```

As defined in the *___init___* function, the model network includes the following layers:

- self.token_embed: it creates an embedding layer that converts token indices (integers) into dense vector representations (embeddings).
- self.pos_embed: this layer create the positional encoding of the input tokens.

- self.blocks: it includes encoder blocks (layers), each with a multi-head self-attention head, a feed-forward network, and the corresponding add & norm components.
- self.ln_f: this layer defines the final layer normalization applied to the transformer's output before passing it into the language modeling head.
- self.lm_head: it defines the language modeling head, i.e., the final layer that maps the hidden representations produced by the transformer into predicted token probabilities.

When an input passes through the *forward* function, it is first converted into token embeddings. Positional embeddings are then added to encode the order of tokens. The resulting representations are sequentially passed through all transformer blocks in the model. Within the *attention head*, the *self.register_buffer* mechanism implements a lower-triangular mask to prevent the model from attending to future tokens during processing.

```python
class Head(nn.Module):
    def __init__(self, n_embed, head_size, block_size, dropout):
        super(Head, self).__init__()
        self.key = nn.Linear(n_embed, head_size, bias=False)
        self.query = nn.Linear(n_embed, head_size, bias=False)
        self.value = nn.Linear(n_embed, head_size, bias=False)
        self.dropout = nn.Dropout(dropout)
        self.register_buffer("tril", torch.tril(torch.ones(block_size, block_size)))

    def forward(self, x):
        B, T, C = x.shape
        k, q, v = self.key(x), self.query(x), self.value(x)
        att = (q @ k.transpose(-2, -1)) / math.sqrt(k.size(-1))
        att = att.masked_fill(self.tril[:T, :T]==0, float('-inf'))
        att = F.softmax(att, dim=-1)
        att = self.dropout(att)
        out = att @ v

        return out
```

The output of the final block is normalized using the last layer normalization and then fed into the language modeling head. At this stage, each token is represented by a hidden vector of size equal to the embedding dimension, and the final layer predicts the probability distribution over the vocabulary for the next token.

```python
class Block(nn.Module):
    def __init__(self, n_embed, n_head, block_size, dropout):
        super(Block, self).__init__()
        self.mh = MultiHead(n_embed, n_head, block_size, dropout)
        self.ff = FeedForward(n_embed, dropout)
        self.ln1 = nn.LayerNorm(n_embed)
        self.ln2 = nn.LayerNorm(n_embed)

    def forward(self, x):
        x_p = self.ln1(x)
        x = x + self.mh(x_p)
        x_p = self.ln2(x)
        x = x + self.ff(x_p)

        return x
```

```python
class FeedForward(nn.Module):
    def __init__(self, n_embed, dropout):
        super(FeedForward, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(n_embed, 4*n_embed),
            nn.GELU(),
            nn.Linear(4*n_embed, n_embed),
            nn.Dropout(dropout)
        )

    def forward(self, x):
        return self.net(x)
```

```python
class MultiHead(nn.Module):
    def __init__(self, n_embed, n_head, block_size, dropout):
        super(MultiHead, self).__init__()
        head_size = n_embed // n_head
        self.heads = nn.ModuleList([
            Head(n_embed, head_size, block_size, dropout) for _ in range(n_head)
        ])
        self.proj = nn.Linear(n_embed, n_embed)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        out = torch.cat([h(x) for h in self.heads], dim=-1)
        proj = self.proj(out)
        return self.dropout(proj)
```

During training, the model compares these predicted logits with the true token IDs using cross-entropy loss, and updates its weights through backpropagation to minimize this loss.

```
num_epochs = 1000
for epoch in range(num_epochs):
    x_batch, y_batch = get_batch(block_size=BLOCK_SIZE, batch_size=BATCH_SIZE)
    _, loss = model(x_batch, y_batch)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    if (epoch + 1) % 100 == 0:
        print(f"Epoch {epoch + 1}/{num_epochs}, Loss: {loss.item(): .4f}")
```

```
Epoch 100/1000, Loss:  1.6484
Epoch 200/1000, Loss:  0.4358
Epoch 300/1000, Loss:  0.1481
Epoch 400/1000, Loss:  0.0896
Epoch 500/1000, Loss:  0.0778
Epoch 600/1000, Loss:  0.0650
Epoch 700/1000, Loss:  0.0572
Epoch 800/1000, Loss:  0.0520
Epoch 900/1000, Loss:  0.0503
Epoch 1000/1000, Loss:  0.0469
```

4.4.1 Evaluation

For evaluation, we provide the model with a starting prompt and ask it to generate the remaining text. Considering the small size of the training data, the generated outputs are reasonably accurate.

```
def generate(prompt="Jalāl ", block_size=16, max_new_tokens=400, temperature=0.8, top_k=50):
    idx = encode(prompt).unsqueeze(0).to(device)
    with torch.no_grad():
        for _ in range(max_new_tokens):
            logits, _ = model(idx[:, -block_size:])
            logits = logits[:, -1, :] / temperature
            if top_k:
                v, _ = torch.topk(logits, min(top_k, logits.size(-1)))
                logits[logits < v[:, [-1]]] = float('-inf')

            probs = F.softmax(logits, dim=-1)
            next_id = torch.multinomial(probs, num_samples=1)
            idx = torch.cat([idx, next_id], dim=1)

    return decode(idx[0].cpu())

print(generate(block_size=BLOCK_SIZE))
```

```
Jalāl al-Dīn Muḥammad Rūmī, or simply Rumi, was a 13th-century poet, Hanafi
faqih, Maturidi theologian, and Sufi mystic born during the Khwarazmian Empire.
Rumi's works are written in his mother tongue, Persian. He occasionally used the
Arabic language and single Turkish and Greek words in his verserserdsiothersiangue, Persian. He occasionally used the
Arabic language and single Turkish and Greek wo
```

Also, we compute the cross-entropy loss, perplexity, accuracy, bit per char (BPC), and distinct scores.

- **Cross-entropy loss:** this metric measures the difference between the predicted probability distribution of a model and the true distribution of the target data. It quantifies how well the model's predicted probabilities match the actual outcomes, with lower values indicating better predictions and less uncertainty.
- **Perplexity:** it measures the model's uncertainty; lower perplexity implies that the model assigns higher probability to the actual next word in the sequence, resulting a more confident and accurate model.
- **Accuracy:** this metric is defined in terms of correct predictions over ground-truth data. However, since the tokens are in terms of characters, accuracy is not a reliable metric in the current evaluations.
- **Bit per char:** BPC measures the average number of bits a model needs to encode or predict each character in the text. Lower BPC indicates better predictive performance and less uncertainty, and it is equivalent to cross-entropy expressed in bits rather than nats.

- **Distinct scores:** these scores quantify diversity in generated text. To compute them, all n-grams of length n in the text are first extracted. The metric then calculates the proportion of unique n-grams relative to the total number of n-grams. A higher score indicates greater diversity, meaning the text is less repetitive.

Table 4.1 indicates the performance of TinyGPT w.r.t. the aforementioned evaluation metrics.

Table 4.1: Performance evaluation of TinyGPT

Cross-Entropy Loss	**Perplexity**	**Accuracy (%)**	**BPC (bits)**	**Distinct-1**	**Distinct-2**
0.0399	1.04	98.48	0.058	0.113	0.432

LLM Fine-tuning

Foundation large language models (LLMs) are trained on vast corpora of data. While they achieve strong overall performance, they often struggle with tasks where the data distribution differs significantly from their training set. Fine-tuning is a crucial technique to address this limitation [10].

Fine-tuning is the process of taking updating the parameters of a pre-trained model by training the model on a dataset specific to the task. Figure 5.1 shows the overall workflow of fine-tuning an LLM.

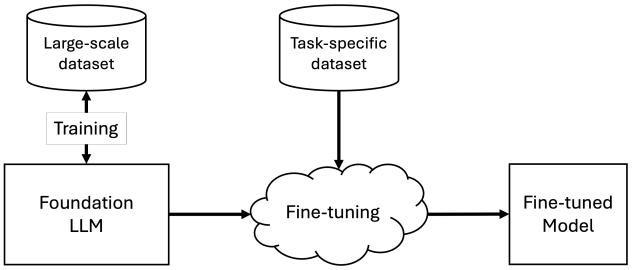


Figure 5.1: Overall workflow of fine-tuning.

5.1 Implementation

In this section, we fine-tune a small and GPU-friendly LLM, namely **Qwen2.5 0.5B-Instruct**. The complete implementation script is available on GitHub.

The fundamental components in fine-tuning a model using Hugging Face application programming interface (API) [2] are *tokenizer*, *foundation model*, *training arguments, (hyperparameters)*, and *data collator*, and *trainer API*.

```
from transformers import AutoTokenizer                    # loads tokenizer for the chosen model
from transformers import AutoModelForCausalLM             # loads a causal language model
from transformers import TrainingArguments                # defines all hyperparameters for training
from transformers import DataCollatorForLanguageModeling  # prepares batches for training
from transformers import Trainer                          # is the Hugging Face API for fine-tuning
```

Tokenizer is responsible for tokenizing the inputs into tokens and encoding them to the corresponding token IDs. Each foundation model has its own tokenizer, developed based on the pre-defined vocabulary (or dictionary) for the model. For loading both tokenizer and model, we define a checkpoint w.r.t. the foundation model we are going to exploit for fine-tuning. Here, we have *checkpoint = "Qwen/Qwen2.5-0.5B-Instruct"*.

```
# fast tokenizer is faster and backed by Rust (systems programming language)
tokenizer = AutoTokenizer.from_pretrained(checkpoint, use_fast=True)

# some models do not own a dedicated padding token; thus, we set it manually
# using end-of-sequence (eos) token to avoid errors
tokenizer.pad_token = tokenizer.eos_token
```

Truncation and padding are essential configurations that must be specified for the tokenizer. To achieve this, a dedicated function (e.g., *tokenization_fn*) is typically defined to set these parameters accordingly. Within this function, the *max_length* parameter plays a key role, as it determines the sequence length used for both truncation and padding.

```
def tokenization_fn(batch):
    out = tokenizer(batch['text'],
                    truncation=True,
                    padding="max_length",
                    max_length=1024,
                   return_tensors=None)
    out["labels"] = out["input_ids"].copy()

    return out

token_data = data.map(tokenization_fn, batched=True, remove_columns=["text"])
token_data
```

Next, we need to load the model from the pre-defined checkpoint.

```
model = AutoModelForCausalLM.from_pretrained(
    checkpoint, device_map="auto", torch_dtype="auto"
)
```

For fine-tuning the loaded model, training arguments must be properly defined. In this regard, we have

- **output_dir**: the directory where checkpoints are saved.
- **per_device_train_batch_size:** keeps virtual random access memory (VRAM) usage low.
- **gradient_accumulation_steps:** simulates larger effective batch size without increasing VRAM.
- **num_train_epochs:** number of passes over the dataset for fine-tuning.
- **learning_rate:** learning rate.
- **logging_steps:** number of steps for logging loss.
- **save_steps:** number of steps to save checkpoints.

```
args = TrainingArguments(
    output_dir='output_dir',
    per_device_train_batch_size=2,
    gradient_accumulation_steps=8,
    num_train_epochs=3,
    learning_rate=1e-4,
    logging_steps=10,
    save_steps=1000
)
```

The data collator handles padding and batching. It takes a list of individual data samples and organizes them into a single and consistent batch using padding, creating attention masks, and handling special tokens.

```
collator = DataCollatorForLanguageModeling(tokenizer, mlm=False) # not a maske language model (MLM) task
# collator = DataCollatorForLanguageModeling(tokenizer, model=model, padding=True) # if padding is not set for tokenizer
```

Finally, we define the *trainer* and perform the fine-tuning.

```
trainer = Trainer(
    model=model,
    args=args,
    train_dataset=token_data,
    data_collator=collator
)
trainer.train()
```

Evaluation

To evaluate the performance of the fine-tuned model, we exploit perplexity, bilingual evaluation understudy (BLEU) [11], and recall-oriented understudy for gisting evaluation (ROUGE) [12].

- **Perplexity:** it measures the model's uncertainty; lower perplexity implies that the model assigns higher probability to the actual next word in the sequence, resulting a more confident and accurate model.
- **BLEU:** this metric evaluates the quality of machine-translated text by comparing it to human-created reference translations. To this end, it computes the overlap of n-grams between the machine-translated text and the reference translation.
- **ROUGE:** it calculates precision, recall, and F1 score to quantify the overlap (n-grams) in words, phrases, and sequences between the machine-translated text and the reference translation.

Table 5.1 indicates the corresponding results. It is worth noting that achieving a highly efficient model requires fine-tuning on an appropriately selected dataset with a sufficient number of samples. However, the objective of this chapter is limited to reviewing the fine-tuning mechanisms in LLMs. Consequently, the resulting model performance may not be fully optimized.

Table 5.1: Performance evaluation of the fine-tuned model

PPL	**BLEU**					**ROUGE**			
	bleu	**unigrams**	**bigrams**	**trigrams**	**quadgrams**	**rouge1**	**rouge2**	**rougeL**	**rougeLSum**
1.1137	0.0440	0.0520	0.0480	0.0419	0.0358	0.1162	0.1000	0.1162	0.1162

Parameter-efficient Fine-tuning

Reinforcement Learning from Human Feedback

Retrieval-Augmented Generation

Agentic AI

References

1. A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin, "Attention is all you need," *Advances in Neural Information Processing Systems*, vol. 30, 2017. [Online]. Available: https://arxiv.org/abs/1706.03762

2. Hugging Face, http://huggingface.co/.

3. LangChain, https://www.langchain.com/.

4. Pinterest, https://www.pinterest.com/.

5. J. Devlin, M.-W. Chang, K. Lee, and K. Toutanova, "Bert: Pre-training of deep bidirectional transformers for language understanding," in *North American Chapter of the Association for Computational Linguistics*, 2019. [Online]. Available: https://api.semanticscholar.org/CorpusID:52967399

6. Y. Liu, M. Ott, N. Goyal, J. Du, M. Joshi, D. Chen, O. Levy, M. Lewis, L. Zettlemoyer, and V. Stoyanov, "Roberta: A robustly optimized bert pretraining approach," 2019. [Online]. Available: https://api.semanticscholar.org/CorpusID:198953378

7. T. B. Brown, B. Mann, N. Ryder, and M. Subbiah*, et al.*, "Language models are few-shot learners," 2020. [Online]. Available: https://arxiv.org/abs/2005.14165

8. A. Chowdhery, S. Narang, J. Devlin, M. Bosma, G. Mishra, A. Roberts, P. Barham, H. W. Chung, C. Sutton, and S. Gehrmann*, et al.*, "Palm: Scaling language modeling with pathways," 2022. [Online]. Available: https://arxiv.org/abs/2204.02311

9. H. Touvron, T. Lavril, and G. Izacard*, et al.*, "Llama: Open and efficient foundation language models," 2023. [Online]. Available: https://arxiv.org/abs/2302.13971

10. M. R. J, K. VM, H. Warrier, and Y. Gupta, "Fine tuning llm for enterprise: Practical guidelines and recommendations," 2024. [Online]. Available: https://arxiv.org/abs/2404.10779

11. K. Papineni, S. Roukos, T. Ward, and W.-J. Zhu, "Bleu: a method for automatic evaluation of machine translation," in *Proceedings of the 40th Annual Meeting on Association for Computational Linguistics*. USA: Association for Computational Linguistics, 2002, p. 311–318. [Online]. Available: https://doi.org/10.3115/1073083.1073135

12. C.-Y. Lin, "Rouge: A package for automatic evaluation of summaries," in *Annual Meeting of the Association for Computational Linguistics*, 2004. [Online]. Available: https://api.semanticscholar.org/CorpusID:964287