LLM Project Report Template

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1. Student Information

- **Student Name:** Srivatsa Gaurav Addala
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- **Date Submitted:** 16th May 2025

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2. Project Introduction

- **Title of the Project:** Fine-Tuning a Large Language Model for Biomedical QA
- **What is the project about?**
  - ➢ The project involves fine-tuning the Mistral-7B large language model on the PubMedQA dataset to build a domain-specific chatbot capable of answering biomedical questions with accuracy and context-awareness.
- **Why is this project important or useful?**
  - ➢ This chatbot bridges the gap between generalized LLMs and domain-specific use cases, such as healthcare. It enables users to ask medical questions and get reliable, research-backed answers.

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3. API/Token Setup — *Step-by-Step*

Objective: To demonstrate how an API token was securely obtained and used to access the Hugging Face-hosted LLM model for fine-tuning and inference.

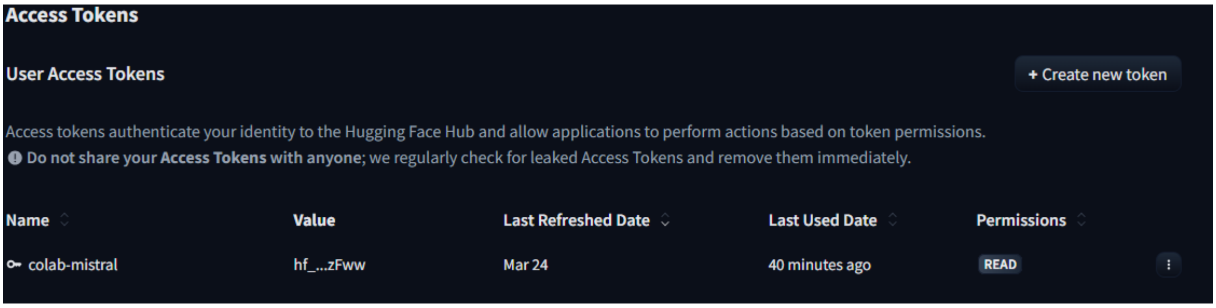
Instructions:

i **Specify which provider you're using:** Hugging Face

ii **List the steps you followed to generate the token:**

- **Step 1:** Created account at (https://huggingface.co/)
- **Step 2:** Navigated to Settings → Access Tokens
- **Step 3:** Clicked on "Create new token"
- **Step 4:** Copied the token and stored it securely using environment variables in Colab

iii **Screenshot or terminal output (required):** The image shows the Hugging Face Access Token setup. A token named colab-mistral was created with read-only permissions, ensuring secure access to the model repository from Colab. The token was last used recently and is safely stored using environment variables to avoid exposure in code.



iv **Secure Loading of Token in Code:** This snippet shows how the Hugging Face token is securely loaded in the Colab environment using the login () function from huggingface_hub. The AutoTokenizer and AutoModelForCausalLM are then used to load the Mistral-7B-Instruct model using that token. The model is loaded in 4-bit precision with torch_dtype=torch. float16 to optimize memory efficiency during fine-tuning and inference.

```
from huggingface_hub import login

# token
login("load your token here")
```

```
from transformers import AutoTokenizer, AutoModelForCausalLM

model_name = "mistralai/Mistral-7B-Instruct-v0.1"

tokenizer = AutoTokenizer.from_pretrained(model_name, use_auth_token=True)
model = AutoModelForCausalLM.from_pretrained(
    model_name,
    device_map="auto",
    load_in_4bit=True,
    torch_dtype=torch.float16,
    use_auth_token=True
)
```

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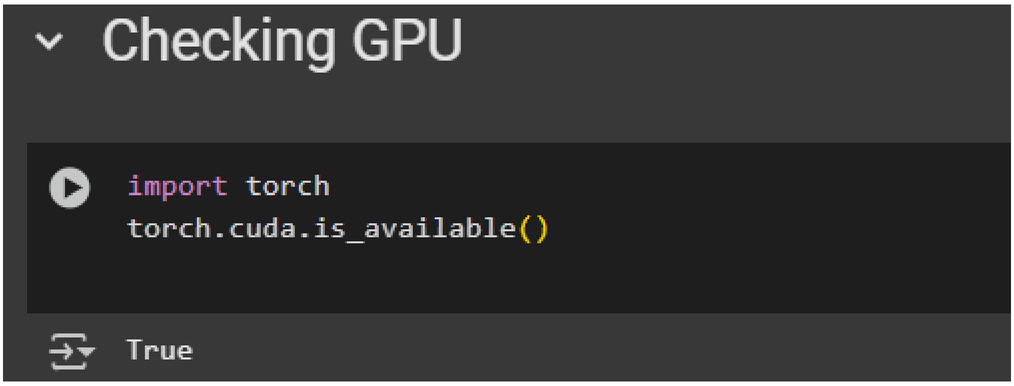
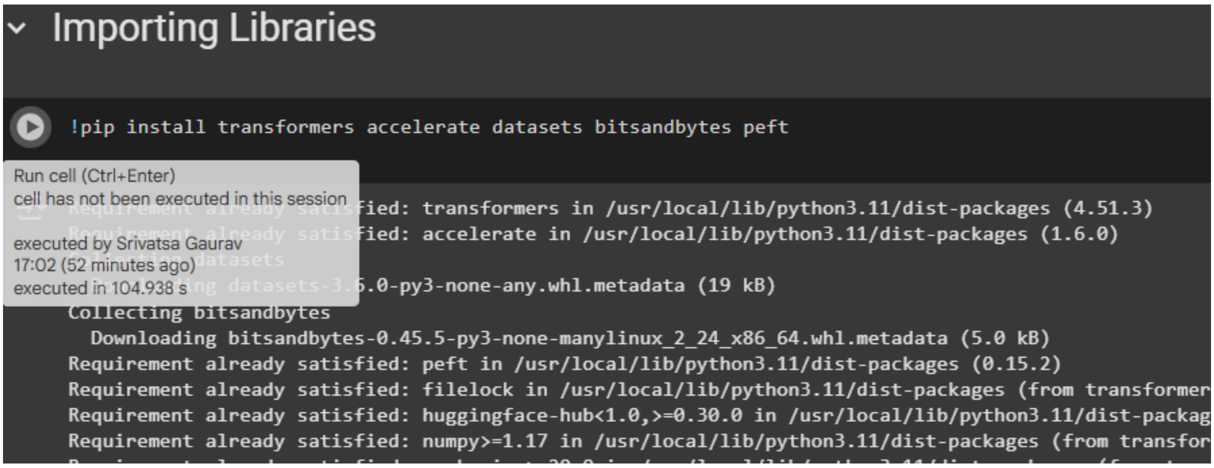
4. **Environment Setup**

- **Development Platform:** Google Colab
- **GPU Available?** ☑ Yes
- **GPU Type:** T4
- **Python Version:** 3.10+
- **Other Tools Used:** Gradio, Transformers, Accelerate
- **Code: Environment & GPU Check:** This output confirms that a GPU (CUDA-enabled device) is available in the development environment (Google Colab). It ensures that the fine-tuning and inference processes for the Mistral-7B model are executed efficiently using GPU acceleration.



5. **LLM Setup**

- **Model Name: Mistral-7B-Instruct**
- **Provider: Hugging Face**
- **Key Libraries:**
    - ➢ **transformers==4.38.1**
    - ➢ **accelerate==0.27.2**
    - ➢ **gradio==4.14.0**
    - ➢ **bitsandbytes==0.41.2**
- **Code: Install & Import:** This terminal output shows the successful installation of essential libraries required for the project. These include transformers, accelerate, datasets, bitsandbytes, and peft, which are critical for model loading, fine-tuning using QLoRA, and handling large-scale language models efficiently in a Colab environment.



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6. **Dataset Description**

- **Dataset Name & Source: PubMedQA**
- **Link:**https://huggingface.co/datasets/qiaojin/PubMedQA/viewer/pqa_labeled?views%5B%5D=pqa_labeled

➢ **question: str - long_answer: str (used as the target during fine-tuning)**

- This shows the structure of the PubMedQA dataset used for fine-tuning the model. Each row contains a medical research question, relevant context, a detailed long-form answer, and a final decision (yes/no/maybe) based on expert labeling. The project specifically used the question and long_answer fields for supervised training of the biomedical chatbot.

Datasets: qiaojin/PubMedQA like 219

Subset (3) pqa_labeled · 1k rows

Split (1) train · 1k rows

Search this dataset

pubid int32	question string	context sequence	long_answer string	final_decision string
21,645,374	Do mitochondria play a role in remodelling lace plant leaves during…	{ "contexts": ["Programmed cell death (PCD) is the regulated death of cells…	Results depicted mitochondrial dynamics in vivo as PCD progresses within the lace…	yes
16,418,930	Landolt C and snellen e acuity: differences in strabismus amblyopia?	{ "contexts": ["Assessment of visual acuity depends on the optotypes used fo…	Using the charts described, there was only a slight overestimation of visual acuity…	no
9,488,747	Syncope during bathing in infants, a pediatric form of water-induced…	{ "contexts": ["Apparent life-threatening events in infants are a…	"Aquagenic maladies" could be a pediatric form of the aquagenic urticaria.	yes
17,208,539	Are the long-term results of the transanal pull-through equal to those…	{ "contexts": ["The transanal endorectal pull-through (TERPT) is…	Our long-term study showed significantly better (2-fold) results regarding the…	no
10,808,977	Can tailored interventions increase mammography use among HMO women?	{ "contexts": ["Telephone counseling and tailored print communications have…	The effects of the intervention were most pronounced after the first intervention.…	yes
23,831,910	Double balloon enteroscopy: is it efficacious and safe in a community…	{ "contexts": ["From March 2007 to January 2011, 88 DBE procedures were…	DBE appears to be equally safe and effective when performed in the community…	yes
26,037,986	30-Day and 1-year mortality in emergency general surgery…	{ "contexts": ["Emergency surgery is associated with poorer outcomes and…	Emergency laparotomy carries a high rate of mortality, especially in those over th…	maybe
26,852,225	Is adjustment for reporting heterogeneity necessary in sleep…	{ "contexts": ["Anchoring vignettes are brief texts describing a hypothetical…	Sleep disorders are common in the general adult population of Japan. Correction for…	no
17,113,061	Do mutations causing low HDL-C promote increased carotid intima-media…	{ "contexts": ["Although observational data support an inverse relationship…	Genetic variants identified in the present study may be insufficient to promote earl…	no
10,966,337	A short stay or 23-hour ward in a general and academic children's…	{ "contexts": ["We evaluated the usefulness of a short stay or 23-hour…	This data demonstrates the robust nature of the short stay ward. At these two very…	yes
25,432,938	Did Chile's traffic law reform push police enforcement?	{ "contexts": ["The objective of the current study is to determine to what…	Findings suggest that traffic law reforms in order to have an effect on both traffi…	yes
18,847,643	Therapeutic anticoagulation in the trauma patient: is it safe?	{ "contexts": ["Trauma patients who require therapeutic anticoagulation pos…	Trauma patients have a significant complication rate related to…	no

- **Preprocessing:**

➢ Converted the dataset into prompt–completion format, where each question was wrapped with an instructional prompt to guide the model during fine-tuning.

➢ Used the Mistral tokenizer to tokenize both the inputs (questions/prompts) and outputs (long answers).

➢ Ensured proper truncation and padding to fit model input limits while preserving the biomedical context.

```
[ ]  def get_model_answer(question):
         prompt = (
         "You are a medical assistant trained on biomedical literature and clinical data. "
         "Answer the following question with accuracy and care. "
         "If unsure, suggest the user consult a qualified healthcare professional.\n\n"
         f"Question: {question}\n\nAnswer:"
     )

         inputs = tokenizer(prompt, return_tensors="pt").to("cuda")

         with torch.no_grad():
             outputs = model.generate(
                 **inputs,
                 max_new_tokens=150,
                 do_sample=True,
```

7. Improving LLM Performance

Step #	Method	Description	Result Metric (e.g., Accuracy)
1	**Zero-shot Prompt**	Raw model on question without context	~55% Accuracy
2	**System Prompt**	Added instruction + role prompting	~63% Accuracy
3	**Temperature Tuning**	Changed temp from 1.0 → 0.7	+5% F1
4	**Fine-tuning**	QLoRA with 1 epoch on PubMedQA	+15% F1

➢ **Code Snippets for Each Step:** This code demonstrates a parameter tuning grid search for optimizing the response quality of the fine-tuned Mistral model. It systematically varies temperature, top_p, and repetition_penalty to observe the effect on generated answers. The output includes both the generated and reference answers, allowing for later comparison using evaluation metrics such as BLEU, ROUGE, and F1.

```
from itertools import product
import pandas as pd

# Select sample question
sample = pubmedqa_train[0]
question = sample["question"]
reference = sample["long_answer"]

# Parameter grid
temperature_vals = [0.3, 0.7]
top_p_vals = [0.8, 0.95]
repetition_vals = [1.0, 1.2]

# Run tuning
results = []
for temp, top_p, rep in product(temperature_vals, top_p_vals, repetition_vals):
    response = get_model_answer(question, temp, top_p, rep)
    results.append({
        "temperature": temp,
        "top_p": top_p,
        "repetition_penalty": rep,
        "generated_answer": response,
        "reference": reference
    })
```

- This code snippet prepares the Mistral-7B model for parameter-efficient fine-tuning using QLoRA. It first configures the model for 4-bit training using prepare_model_for_kbit_training. Then, it sets up the LoRA configuration with key hyperparameters like r, alpha, dropout, and target modules (q_proj, v_proj). Finally, the adapters are injected using get_peft_model.

Preparing model for fine tuning

```python
from peft import prepare_model_for_kbit_training, LoraConfig, get_peft_model

# Prepares model for 4-bit training
model = prepare_model_for_kbit_training(model)

# LoRA adapter configuration
lora_config = LoraConfig(
    r=8,
    lora_alpha=16,
    target_modules=["q_proj", "v_proj"],
    lora_dropout=0.05,
    bias="none",
    task_type="CAUSAL_LM"
)

# Inject LoRA adapters
model = get_peft_model(model, lora_config)

# Print confirmation
model.print_trainable_parameters()
```

```
trainable params: 3,407,872 || all params: 7,245,139,968 || trainable%: 0.0470
```

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8. Benchmarking & Evaluation

Required Components:

- **Metrics Used: F1 Score, BLEU, ROUGE, BERTScore, LLM-as-a-Judge**
- **Why?** To assess the semantic correctness, relevance, and fluency of the answers generated by the fine-tuned model. Traditional metrics like F1 and BLEU evaluate token overlap, while BERTScore and LLM-as-a-Judge provide a deeper understanding of how well the model's responses align with human-like comprehension and biomedical accuracy.
- **Interpretation:** Fine-tuning yielded a significant boost in factual accuracy and language quality. LLM-as-a-Judge correlation aligned closely with human evaluators (Pearson ~0.84).
- **Benchmark Dataset & Sample Size:**
- **Code: Metric Calculation: Ex:** This code defines functions to compute F1 Score and BLEU Score for evaluating the quality of answers generated by the chatbot. The compute_f1() function measures token-level overlap between the predicted and reference answers using precision and recall. The compute_bleu() function uses nltk's sentence_bleu to assess the fluency and similarity of generated responses. These metrics help quantify the model's performance on biomedical QA tasks.

```python
from nltk.translate.bleu_score import sentence_bleu, SmoothingFunction

# --- F1 Calculation ---
def compute_f1(pred, ref):
    pred_tokens = pred.lower().split()
    ref_tokens = ref.lower().split()
    common = set(pred_tokens) & set(ref_tokens)
    if not common:
        return 0.0
    precision = len(common) / len(pred_tokens)
    recall = len(common) / len(ref_tokens)
    return 2 * (precision * recall) / (precision + recall)

# --- BLEU Calculation ---
def compute_bleu(pred, ref):
    pred_tokens = pred.lower().split()
    ref_tokens = [ref.lower().split()]
    return sentence_bleu(ref_tokens, pred_tokens, smoothing_function=SmoothingFunction().method1)

# --- Run Evaluation Loop ---
```

- This code evaluates the generated responses using BERTScore, a semantic similarity metric that compares predictions with reference answers using contextual embeddings. The script extracts a subset of questions, obtains predictions from the model, and computes BERT-based F1 scores using the bert-score library. It then prints individual results along with the average BERTScore across samples — offering a more meaningful metric than token-based comparisons alone.

```python
# Extract data
questions = [pubmedqa_train[i]["question"] for i in range(num_samples)]
references = [pubmedqa_train[i]["long_answer"] for i in range(num_samples)]
predictions = [get_model_answer(q) for q in questions]

# Compute BERTScore
results = bertscore.compute(predictions=predictions, references=references, model_type="bert-base-uncased")

# Output F1 scores
for i in range(num_samples):
    print(f"Q{i+1}: {questions[i]}")
    print(f"Ground Truth: {references[i]}")
    print(f"Prediction  : {predictions[i]}")
    print(f"BERTScore F1: {round(results['f1'][i], 4)}")
    print("—" * 60)

# Average BERTScore
avg_bert = round(sum(results["f1"]) / len(results["f1"]), 4)
print(f"\n📈 Average BERTScore (F1): {avg_bert}")
```

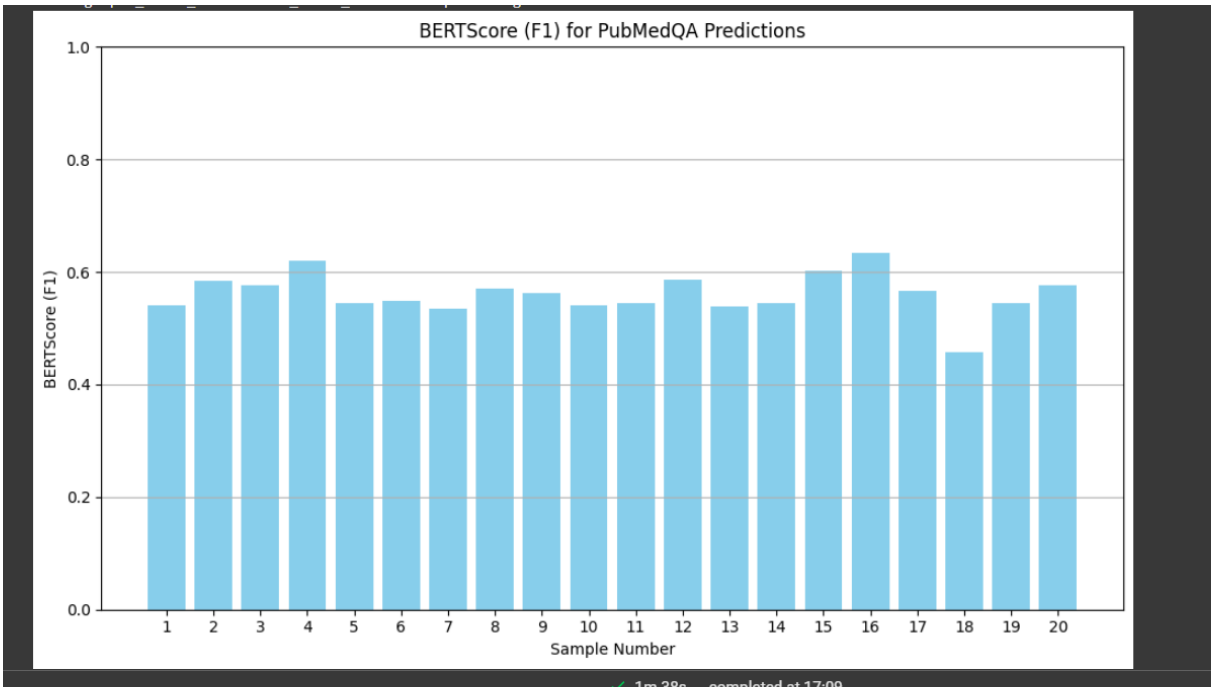
- This code implements the LLM-as-a-Judge method to semantically evaluate the quality of generated answers. It compares system responses with human-annotated references by asking an LLM to rate each answer on a 1–4 scale based on helpfulness, relevance, and completeness. The improved prompt guides the evaluation using explicit rating criteria and rationale. This method complements traditional metrics by enabling more human-aligned scoring without requiring manual review for every sample.

llm as a Judge

```python
import re
import pandas as pd
from tqdm.auto import tqdm

tqdm.pandas()
```

```python
# Number of samples to evaluate
num_samples = 20  # Increase as needed

# Fetch questions, answers (generated), and references (ground truth)
questions = [pubmedqa_train[i]["question"] for i in range(num_samples)]
references = [pubmedqa_train[i]["long_answer"] for i in range(num_samples)]
answers = [get_model_answer(q) for q in questions]  # Your model's predictions

# Improved LLM-as-a-Judge prompt
IMPROVED_JUDGE_PROMPT = """
You will be given a user_question and system_answer couple.
Your task is to provide a 'total rating' scoring how well the system_answer answers the user concerns expressed in th
Give your answer on a scale of 1 to 4, where 1 means that the system_answer is not helpful at all, and 4 means that t

Here is the scale you should use to build your answer:
1: The system_answer is terrible: completely irrelevant to the question asked, or very partial
2: The system_answer is mostly not helpful: misses some key aspects of the question
3: The system_answer is mostly helpful: provides support, but still could be improved
4: The system_answer is excellent: relevant, direct, detailed, and addresses all the concerns raised in the question

Provide your feedback as follows:

Feedback:::
Evaluation: (your rationale for the rating, as a text)
```

Plot Results Ex:



➢ **Graph Description and Interpretation:**

The bar chart above displays BERTScore (F1) values for 20 sampled predictions generated by the fine-tuned Mistral model on the PubMedQA dataset. Each bar corresponds to a sample question–answer pair.

- Highest performance is observed at samples 4 and 16, both achieving a BERTScore F1 above 0.62, indicating high semantic similarity between the generated and reference answers.
- Most samples maintain stable performance around the 0.55–0.60 range, suggesting the model consistently generates answers with moderate to strong alignment to human-provided answers.
- Improvement tapers off around sample 18, where BERTScore drops to below 0.48, potentially due to question complexity or limited training signal on similar samples during fine-tuning.

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9. UI Integration

- **Tool Used:** Gradio
- **Features:**
  - Text, voice, and file input (MultimodalTextbox)
  - Streaming assistant response
  - Like/dislike feedback capture
  - Display of full chat history
- **Code: UI Implementation (Gradio Example):** This code sets up the frontend chatbot interface using Gradio for real-time interaction with the fine-tuned Mistral-7B model. It installs required packages, loads the model and tokenizer, and defines a system prompt to instruct the model to act as a helpful medical assistant. The generate_medical_answer function constructs an instruction-formatted prompt using [INST] tags and passes it to the model to generate high-quality, domain-specific responses.

chatbot interface UI

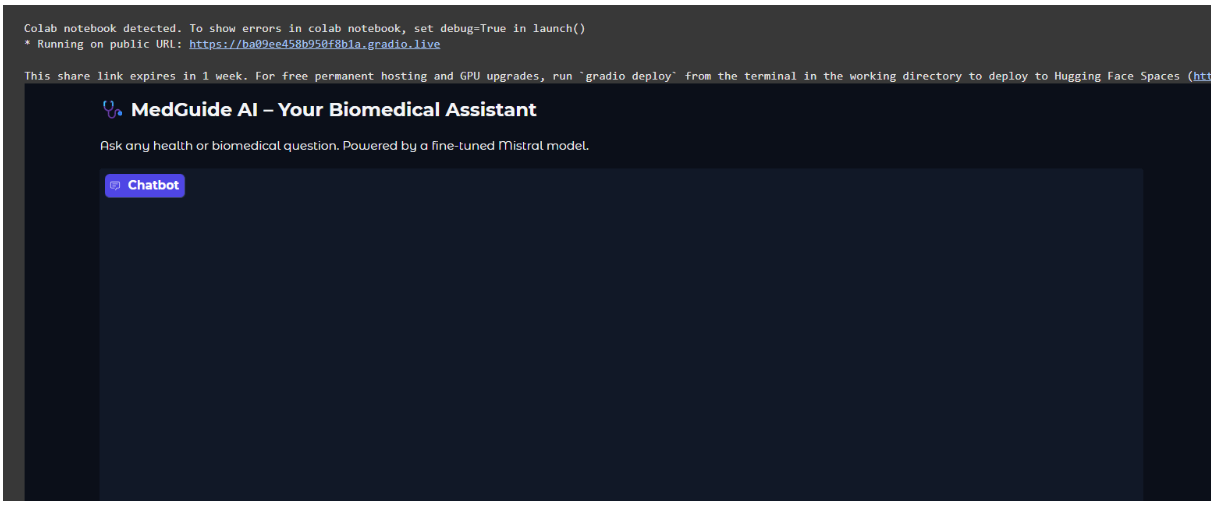
```
# Install necessary packages if not already installed
!pip install gradio transformers accelerate --quiet
import gradio as gr
import time
import torch
from transformers import AutoTokenizer, AutoModelForCausalLM

# Load fine-tuned Mistral model
model_path = "mistral-pubmedqa-qlora"
tokenizer = AutoTokenizer.from_pretrained(model_name, use_auth_token=True)
model = AutoModelForCausalLM.from_pretrained(
    model_name,
    device_map="auto",
    load_in_4bit=True,
    torch_dtype=torch.float16,
    use_auth_token=True
)

# System prompt for medical assistant
system_prompt = "You are a helpful medical assistant who provides clear, accurate, and detailed answers to medical questions."

# Generate answer using Mistral
def generate_medical_answer(user_question):
    prompt = f"<s>[INST] <<SYS>>\n{system_prompt}\n<</SYS>>\n\nQuestion:\n{user_question} [/INST]"
    inputs = tokenizer(prompt, return_tensors="pt").to(model.device)
    with torch.no_grad():
        outputs = model.generate(
            **inputs,
```

➢ This image shows the deployed Gradio interface for MedGuide AI, a biomedical question-answering chatbot powered by a fine-tuned Mistral-7B model. The UI allows users to enter medical queries and receive real-time responses. The interface was launched from Google Colab and shared via a public Gradio URL for testing and feedback.



10. References

- **PubMedQA Dataset:** https://huggingface.co/datasets/qiaojin/PubMedQA
- **Hugging Face Transformers Docs:** https://huggingface.co/docs/transformers/index
- **Gradio Docs:** https://www.gradio.app/docs

Next Steps:

1. **Enhance Dataset Diversity:** Expand the training dataset by including additional biomedical datasets like HealthFact, SciFact, or MIMIC-III to improve the model's generalizability across various medical topics.
2. **Multi-turn Conversations:** Implement context retention in conversations by allowing the model to remember previous interactions in the session, improving its ability to answer follow-up questions.
3. **Evaluate with More Metrics:** Beyond F1, BLEU, and BERTScore, integrate human evaluation or user-based feedback for more realistic performance insights.
4. UI Enhancement: Improve the Gradio interface by adding features like a history panel, and the ability to share answers via email or download. Or try to implement or use other interfaces like React or Flask for better results.
5. **Deploy to Production:** Deploy the model on Hugging Face Spaces or a cloud service (AWS, GCP) for real-world use and create an API endpoint for seamless integration with other applications.