MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant

A PROJECT REPORT

Submitted by

MASRUK HABIB

92100103165

PUVANENTHIRARAJAH

92100103168

BACHELOR OF TECHNOLOGY

in

Computer Engineering

Faculty of Engineering & Technology

Marwadi University, Rajkot

April, 2025

Major Project-II (01CE0807)

Department of Computer Engineering

Faculty of Engineering & Technology

Marwadi University

A.Y. 2024-25

CERTIFICATE

This is to certify that the project report submitted along with the project entitled **MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant** has been carried out by **Masruk Habib** (92100103165), **Puvanenthirarajah** (92100103168) under my guidance in partial fulfilment for the degree of Bachelor of Technology in Computer Engineering, 8th Semester of Marwadi University, Rajkot during the academic year 2024-25.

Ravikumar R N	Dr. Krunal Vaghela
Asst. Professor (Internal Guide)	Professor & Head
Department of Computer Engineering	Department of Computer Engineering

Major Project-II (01CE0807)

Department of Computer Engineering

Faculty of Engineering & Technology

Marwadi University

A.Y. 2024-25

CERTIFICATE

This is to certify that the project report submitted along with the project entitled **MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant** has been carried out by **Masruk Habib** (92100103165) under my guidance in partial fulfilment for the degree of Bachelor of Technology in Computer Engineering, 8th Semester of Marwadi University, Rajkot during the academic year 2024-25.

Ravikumar R N	Dr. Krunal Vaghela
Asst. Professor (Internal Guide)	Professor & Head
Department of Computer Engineering	Department of Computer Engineering

Major Project-II (01CE0807)

Department of Computer Engineering

Faculty of Engineering & Technology

Marwadi University

A.Y. 2024-25

CERTIFICATE

This is to certify that the project report submitted along with the project entitled **MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant** has been carried out by **Puvanenthirarajah** (92100103168) under my guidance in partial fulfilment for the degree of Bachelor of Technology in Computer Engineering, 8th Semester of Marwadi University, Rajkot during the academic year 2024-25.

Ravikumar R N	Dr. Krunal Vaghela
Asst. Professor (Internal Guide)	Professor & Head
Department of Computer Engineering	Department of Computer Engineering

Major Project-II (01CE0807)

Department of Computer Engineering

Faculty of Engineering & Technology

Marwadi University

A.Y. 2024-25

DECLARATION

We hereby declare that the **Major Project-II (01CE0807)** report submitted along with the Project entitled **MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant** submitted in partial fulfilment for the degree of Bachelor of Technology in Computer Engineering to Marwadi University, Rajkot, is a bonafide record of original project work carried out by me / us at Marwadi University under the supervision of **Prof. Ravikumar R N** and that no part of this report has been directly copied from any students reports or taken from any other source, without providing due reference.

	Name of the Student	Sign of Student
1	Masruk Habib	_____
2	Puvanenthirarajah	_____

Acknowledgement

We express our deepest gratitude to the Almighty for His divine blessings, which have guided us in successfully completing this major project.

We extend our heartfelt appreciation to Prof. Ravikumar R. N., Assistant Professor, Marwadi University, Rajkot, Gujarat, for his invaluable guidance, unwavering support, and insightful mentorship throughout this project. His expertise in Machine Learning and his dedication to academic excellence have been a constant source of inspiration. His meticulous supervision, constructive feedback, and continuous encouragement played a pivotal role in shaping the success of this endeavour.

Our sincere gratitude also goes to Dr. Kurnal Vagela, Head of the Department of Computer Engineering, for his support and encouragement. We are equally thankful to the esteemed faculty members and staff of the Computer Engineering Department at Marwadi University for their cooperation and assistance, which contributed significantly to the smooth progress of our work.

Furthermore, we deeply appreciate the contributions of all individuals who supported us through constructive feedback, encouragement, and practical assistance. Your collective efforts have been instrumental in bringing this project to completion.

This project would not have been possible without the unwavering support, guidance, and collaboration of everyone involved, for which we are profoundly grateful.

Abstract

Polypharmacy, the concurrent use of multiple medications, increases the risk of adverse drug interactions, leading to severe side effects or reduced therapeutic efficacy. Traditional drug interaction systems rely on static databases that lack adaptability to emerging medications and complex interaction patterns. MediGuard AI addresses these limitations by leveraging large language models (LLMs) with retrieval-augmented generation (RAG) to enhance drug interaction prediction and personalized side effect analysis. The system is fine-tuned on comprehensive medical datasets, including DrugBank and SIDER, enabling real-time identification of harmful drug combinations, risk scoring, and safer medication recommendations based on patient-specific data such as age, medical history, and prescriptions. Additionally, MediGuard AI incorporates an interactive RAG-based chat assistant, allowing healthcare providers to query drug interactions, receive context-aware responses, and make informed clinical decisions. By integrating patient demographics and real-time retrieval of medical knowledge, the system enhances drug safety, reduces medication errors, and improves personalized healthcare insights. This research highlights the potential of AI-driven solutions in revolutionizing medication management and patient care.

Keywords*—Polypharmacy, Large Language Models (LLMs), Retrieval-Augmented Generation (RAG), Drug Interaction Prediction, Personalized Healthcare, Adverse Drug Reactions.*

.

List of Figures

Fig 3.1 Work Flow..... 14

Fig 3.2 Top 10 most common DI types..... 18

Fig 3.3 Top DI Types and count..... 19

Fig 3.4 Word Cloud of DDI Type..... 20

Fig 3.5 Histogram of DDI Type..... 20

Fig 3.6 Network Graph (first 500 records) 21

Fig 3.7 Distribution of Top 8 Interactions Types..... 22

Fig 3.8 Bubble chart of DI with total number of DI..... 23

Fig3.9 Merged DDI Type Index..... 24

Fig 3.10 Proportion of Origin DDI Types..... 24

Fig 3.11 Model Steup Phase..... 25

Fig 3.12 RAG based chat Assistance..... 29

Fig 4.1 Result..... 30

Fig 4.2 Evaluation Metrics..... 32

Fig 4.3 training loss and validation loss over epochs 33

Fig 4.4 Home page of MediGuard AI..... 34

Fig 4.5 Medication Information..... 34

Fig 4.6 Analysis Results..... 35

Fig 4.7 Medication Interaction Report..... 35

Fig 4.8 Key Recommendations, Monitoring Schedule..... 36

List of Tables

Table 1.1 Project Management Table..... 7

Table 2.1 Comparison of Key LLM-Based Models for Drug Interaction Prediction.....9

Table 2.3 Literature Review..... 10

Table 3.1 DDI Types..... 15

Table 4.1 Evaluation Metrics..... 31

Abbreviations

LLM	**Large Language Model**
LoRA	**Low Rank Adaptation**
QLoRA	**Quantized LoRA**
ML	**Machine Learning**
SDLC	**Software Development Life Cycle**
DL	**Deep Learning**
LOC	**Line of Code**
TP	**True Positive**
TN	**True Negative**
FP	**False Positive**
FN	**False Negative**
DDI	**Drug-Drug interactions**

Table of Contents

Acknowledgement..... i

Abstract ii

List of Figures iii

List of Tables iv

List of Abbreviations v

Table of Contents vi

Chapter 1 INTRODUCTION 1

1.1 Introduction to Medicated AI..... 1

1.2 Uses of Medicated AI..... 2

1.3 Study Goal..... 2

1.4 Benefits of Medicated AI..... 3

1.5 Motivation for Medicated AI..... 3

1.6 Expected Outcome of Medicated AI..... 4

1.7 Project Management of Medicated AI..... 5

1.7.1. Project Planning..... 5

1.7.2. Development & Implementation..... 5

1.7.3. Testing & Evaluation..... 6

1.7.4. Deployment & Integration..... 6

1.7.5. Monitoring & Optimization..... 6

1.8 Project Management and Finance ….....7

Chapter 2 LITERATURE REVIEW……..... 8

2.1 Related Works..... 8

2.2 Technical Capabilities of LLMs in Drug Interaction Prediction..... 8

2.3 Literature Review.....10

Chapter 3 RESEARCH METHODOLOGY.....13

3.1 Methodology..... 13

3.2 Data Sources & Knowledge Integration.....14

3.3 Drug-to-Drug interactions Types..... 15

3.4 Data Processing 18

3.5 Visualization.....18
3.5.1 Top 10 most common DI types.....18
3.5.2 Top DI Types and count.....19
3.5.3 Word Cloud of DDI Type.....20
3.5.4 Histogram of DDI Type..... 20
3.5.5 Network Graph (first 500 records) 21
3.5.6 Distribution of Top 8 Interactions Types..... 22
3.5.7 Bubble chart of DI with total number of DI..... 23
3.5.8 Merged DDI Type Index..... 24
3.5.9 Proportion of DDI Types..... 24
3.6 Model Training..... 25
3.7 Model Evolution..... 26
3.8 MediGuardAi Chat assistance..... 28
Chapter 4 RESULT AND DISCUSSION..... 30
4.1 Experimental Results & Analysis 30
4.2 Result Graph 31
4.2.1 Line plot comparing training loss and validation loss over epochs..... 32
4.3 Website implementation..... 33
4.3.1 Medication Information.....34
4.3.2 Analysis Results..... 35
4.3.3 Medication Interaction Report, Side Effects Analysis, Key Recommendations, Monitoring Schedule. 35
Chapter 5 CONCLUSION AND FUTURE DIRECTION..... 37
5.1 Summary of the Study..... 37
5.2 Conclusion 37
5.3 Implication for Future Study 38
References 40

CHAPTER 1

INTRODUCTION

1.1 Introduction to Medicated AI

In the evolving landscape of healthcare, artificial intelligence (AI) is playing a crucial role in enhancing medication management, diagnosis, and treatment strategies. "Medicated AI" is a cutting-edge project designed to identify and mitigate drug-to-drug interactions (DDI), ensuring safer medication usage for patients. This system leverages machine learning models and large language models (LLMs) to analyse complex pharmaceutical data, offering accurate risk assessments and recommendations for healthcare professionals.

The project utilizes the Drug-Drug Interaction (DDI) dataset, incorporating multiple DDI types to improve the accuracy of interaction detection. A pre-trained LLaMA 2 7B model powers the analysis, enabling the system to process vast amounts of medical data and provide insightful predictions. The application is built using Django, ensuring a robust and user-friendly platform where users can input medication data for real-time risk evaluation.

By allowing users to select and input medication details, the system analyzes interactions and provides risk assessments tailored to individual patient data. This approach enhances transparency and supports informed decision-making for both healthcare professionals and patients.

Medicated AI has achieved an accuracy of over 85%, demonstrating its effectiveness in predicting and assessing drug interactions. The system has also produced the best validation and training loss graphs, ensuring its reliability in real-world applications. These performance metrics highlight the robustness of the model and its capability to provide precise and actionable insights.

The ultimate goal of Medicated AI is to improve the quality and efficiency of healthcare by reducing adverse drug interactions. By integrating AI-driven insights with medical expertise, the project contributes to safer medication practices, minimizing risks and enhancing patient

outcomes. This innovation marks a significant step towards the future of AI-assisted healthcare, bridging the gap between technology and medical safety.

1.2 Uses of Medicated AI

Medicated AI plays a crucial role in enhancing patient safety and improving healthcare efficiency by leveraging artificial intelligence for drug interaction detection and risk assessment. This system helps healthcare professionals make informed decisions, reducing the chances of adverse drug effects and ensuring safer medication usage. By analyzing patient medication data, it provides personalized recommendations and assists in optimizing treatment plans.

Furthermore, Medicated AI supports medical research and development, enabling researchers to study drug interactions and advance pharmaceutical safety. It can be integrated into hospital databases and electronic health records for real-time monitoring and alert generation, making healthcare systems more efficient. Additionally, medical students and professionals can use it as an educational tool to enhance their understanding of drug interactions and safe prescribing practices. Ultimately, Medicated AI contributes significantly to improving patient well-being and advancing the future of AI-assisted healthcare.

1.3 Study Goal

The primary goal of this study is to develop an AI-powered system that enhances drug safety by accurately detecting and assessing drug-to-drug interactions (DDIs). Medicated AI aims to leverage advanced machine learning and large language models to analyze pharmaceutical data, providing precise risk assessments and medication recommendations. The study focuses on improving healthcare efficiency, reducing adverse drug effects, and supporting medical professionals in making informed decisions. Additionally, it seeks to contribute to pharmaceutical research and education, offering a valuable tool for both researchers and healthcare practitioners. By integrating AI into healthcare systems, this study aims to enhance patient safety, optimize treatment plans, and pave the way for more reliable AI-assisted medical solutions.

1.4 Benefits of Medicated AI

Medicated AI offers numerous benefits in the healthcare sector by improving drug safety and enhancing patient care. One of its key advantages is its ability to accurately detect and analyze drug-to-drug interactions (DDIs), reducing the risk of adverse effects and ensuring safer medication usage. By leveraging machine learning and large language models, the system provides precise risk assessments and personalized medication recommendations, helping healthcare professionals make well-informed decisions.

Additionally, Medicated AI enhances healthcare efficiency by streamlining medication management and reducing human errors in prescribing drugs. Its integration with hospital databases and electronic health records enables real-time monitoring, alert generation, and seamless patient data analysis. This not only improves workflow efficiency but also enhances patient safety by preventing harmful drug combinations.

Furthermore, Medicated AI contributes to pharmaceutical research and education by providing valuable insights into drug interactions and medication effects. Researchers can utilize this system to study new interactions, while medical students and professionals can benefit from it as an educational tool to improve their knowledge of safe prescribing practices.

Ultimately, Medicated AI plays a crucial role in revolutionizing the healthcare industry, reducing medication-related risks, supporting medical research, and enhancing overall patient well-being through AI-driven innovations.

1.5 Motivation for Medicated AI

The increasing complexity of modern medicine, with a vast number of available drugs and their potential interactions, poses significant challenges to healthcare professionals and patients alike. Adverse drug interactions can lead to severe health complications, increased hospitalizations, and even fatalities. Traditional methods of identifying and managing drug interactions rely on manual reviews and outdated databases, making them inefficient and prone to errors.

Medicated AI is motivated by the need to enhance medication safety and optimize healthcare decision-making through artificial intelligence. By leveraging machine learning and large language models, this system aims to provide accurate drug interaction analysis, personalized medication recommendations, and real-time risk assessments. This not only improves patient safety but also aids doctors, pharmacists, and researchers in making data-driven medical decisions.

Furthermore, with the integration of AI into healthcare systems, Medicated AI seeks to bridge the gap between technology and medical practice. Its ability to automate drug interaction detection, integrate with electronic health records, and provide valuable insights into pharmaceutical research makes it a game-changer in the medical field. The project is driven by a vision to minimize medication-related risks, enhance healthcare efficiency, and empower both professionals and patients with reliable AI-driven support.

Ultimately, the motivation behind Medicated AI is to revolutionize medication management, reduce adverse drug effects, and contribute to the broader goal of improving global healthcare outcomes through innovative and intelligent technology.

1.6 Expected Outcome of Medicated AI

Medicated AI is designed to significantly enhance drug safety and healthcare efficiency by accurately identifying and mitigating drug-to-drug interactions (DDIs). The expected outcome of this project is a highly reliable AI-powered system capable of analysing complex pharmaceutical data, providing precise risk assessments, and offering personalized medication recommendations.

One of the key outcomes is the reduction of adverse drug reactions, leading to improved patient safety and fewer medication-related hospitalizations. By integrating AI-driven analysis into healthcare workflows, Medicated AI aims to assist doctors, pharmacists, and researchers in making data-driven decisions, ultimately optimizing prescription accuracy and treatment effectiveness.

Furthermore, the system is expected to seamlessly integrate with hospital databases and electronic health records, enabling real-time monitoring and alert generation for potential drug

interactions. This will streamline healthcare operations, reduce human errors, and enhance overall efficiency in medical institutions.

Another expected outcome is the contribution to pharmaceutical research and medical education. Medicated AI will serve as a valuable tool for researchers studying new drug interactions and for medical students learning about safe prescribing practices. By providing data-driven insights, the system will support the development of new treatment strategies and improved medication management practices.

Overall, Medicated AI is set to revolutionize the healthcare industry by ensuring safer medication use, reducing risks associated with drug interactions, enhancing healthcare decision-making, and ultimately improving patient outcomes through AI-driven innovation.

1.7 Project Management of Medicated AI

The successful implementation of Medicated AI requires a well-structured project management approach, ensuring efficient development, testing, and deployment. This project follows a systematic workflow encompassing planning, execution, monitoring, and optimization to achieve its goals effectively.

1.7.1. Project Planning

- Define clear objectives, including drug-to-drug interaction detection, risk assessment, and AI-powered recommendations.
- Establish a timeline and milestones to track progress efficiently.
- Identify key resources, including data sources (DDI dataset), AI models (LLaMA 2 7B), and the Django framework for application development.

1.7.2. Development & Implementation

- Collect and preprocess pharmaceutical data to ensure model accuracy and reliability.
- Train and fine-tune the AI model using machine learning techniques to achieve optimal performance.

- Develop a user-friendly web application for healthcare professionals and researchers to interact with the system.

1.7.3. Testing & Evaluation

- Conduct rigorous testing, including unit testing, integration testing, and validation against real-world datasets.
- Evaluate model performance based on accuracy, validation loss, and training loss.
- Make necessary improvements to enhance system robustness and reliability.

1.7.4. Deployment & Integration

- Deploy the Medicated AI system within healthcare institutions and integrate it with electronic health records (EHRs).
- Ensure seamless operation with real-time monitoring and alert generation for potential drug interactions.

1.7.5. Monitoring & Optimization

- Continuously monitor system performance and user feedback to refine the model and application.
- Implement updates to improve accuracy, scalability, and overall efficiency.
- Maintain compliance with medical regulations and data privacy standards.

By following this structured project management approach, Medicated AI aims to achieve its objectives efficiently while ensuring a high-impact contribution to the healthcare industry. This systematic execution will help create a robust, AI-powered solution that enhances drug safety and supports medical decision-making.

1.8 Project Management and Finance

Effective project management and financial planning are crucial for the successful execution of any research or development initiative. In this study, project management involves defining clear objectives, setting milestones, and ensuring the systematic implementation of Large language models (LLM) and RAG for MediGuard AI – An Interactive Drug Interaction and Side Effect Predictor using LLMs with RAG based Chat Assistance. Proper task allocation, timeline management, and risk assessment help maintain efficiency and ensure that deliverables are met within the scheduled timeframe. Additionally, financial planning plays a vital role in resource allocation, covering costs related to data acquisition, computational resources, software tools, and web application development. Budget optimization ensures the efficient use of available funds, preventing unnecessary expenses while maximizing output quality. Effective management strategies also include securing funding from grants, institutional support, or research collaborations, which can enhance the projects scope and impact. By maintaining a structured approach to project execution and financial management, this research aims to achieve its objectives within the allocated budget and timeframe while delivering a high-quality, impactful solution.

Table 1.1 Project Management Table

Work	**Time**
Project Initiation	Week 1-2
Research and Data Collection	Week 3-5
Data Preprocessing	Week 6-7
Model Development	Week 8-10
Testing, Evaluation and Implementation	Week 11-15
Reporting and Documentation	Week 15-16
Total	**Week 16**

CHAPTER 2

LITERATURE REVIEW

2.1 Related Works

The integration of large language models (LLMs) into healthcare has opened new avenues for improving drug interaction and side effect prediction. These models leverage vast amounts of biomedical data to provide accurate and comprehensive predictions, enhancing patient safety and clinical decision-making. This response explores the development and application of LLM-based systems for predicting drug interactions and side effects, highlighting their capabilities, challenges, and future directions.

2.2 Technical Capabilities of LLMs in Drug Interaction Prediction

LLMs have demonstrated remarkable capabilities in processing biomedical text and generating predictions. For instance, LEDAP, a framework leveraging LLM-based biotext feature encoding, has shown notable competitiveness in predicting drug-disease associations and drug-drug interactions (DDIs) [1] Similarly, DrugChat, a multi-modal LLM, can analyse molecular structures and user queries to predict drug mechanisms and properties, facilitating interactive exploration [2]. In clinical settings, LLM-based systems can analyze patient data, including medical history and individual characteristics, to predict DDIs and optimize treatment plans [3]. For example, PTB-DDI, a framework combining ChemBerta tokenizer and BiLSTM, achieved high accuracy in predicting DDIs on real-world datasets [4].

The risk of misinformation is a significant concern when using LLMs for drug interaction prediction. As highlighted in Paper 1, patients relying solely on AI-generated advice for self-medication decisions could face safety risks [5]. Regulatory oversight is essential to ensure these tools serve as supplements to professional healthcare guidance rather than replacements. The integration of LLMs with EHRs could revolutionize clinical decision-making. By analyzing comprehensive patient data, these models could provide personalized predictions and recommendations, enhancing treatment safety and efficacy [6].

Table 2.1 Comparison of Key LLM-Based Models for Drug Interaction Prediction

Model Name	Key Features	Performance Metrics
LEDAP	LLM-based biotext feature encoding	Achieved state-of-the-art performance in DBA tasks [1].
KELLM	Knowledge-enhanced LLM with causal chains	Demonstrated state-of-the-art performance in effectiveness and safety metrics [7].
DDI-GPT	Combines LLMs with knowledge graphs	Achieved AUROC of 0.964 on TwoSIDES dataset [8].
DrugChat	Multi-modal LLM for drug mechanisms	Outperformed GPT-4 in generating accurate free-form predictions [2].
ALG-DDI	Multi-scale feature fusion model	Outperformed state-of-the-art models on varying datasets [9].
KnowDDI	Knowledge subgraph learning for interpretability	Achieved state-of-the-art prediction performance with better interpretability [9].
PTB-DDI	ChemBerta tokenizer and BiLSTM	Achieved AUC-ROC of 0.997 on BIOSNAP dataset [4].
R2-DDI	Relation-aware feature refinement	Improved DDI prediction performance across multiple datasets [10].

Large language models have the potential to transform drug interaction and side effect prediction by providing accurate, interpretable, and interactive solutions. While challenges such as data quality, misinformation, and regulatory oversight remain, ongoing advancements in model architecture, knowledge integration, and clinical applications are paving the way for their effective integration into healthcare systems. As these models continue to evolve, they will play an increasingly important role in enhancing patient safety and improving clinical outcomes.

2.3 Literature Review

Table 2.3 Literature Review

Ref.	Dataset	Result	Methods Used	Limitations
[11]	TwoSIDES benchmark dataset for DDI prediction. FDA Adverse Event Reporting System for zero-shot prediction.	DDI-GPT achieved 0.964 AUROC on TwoSIDES dataset. Improved zero-shot prediction accuracy to 0.84 AUROC.	Combines knowledge graphs and large language models. Utilizes feature attribution methods for explainability.	-
[12]	-	Initial results are promising for DDI prediction. Further refinement and larger datasets needed for accuracy.	Large language models for DDI prediction . Natural language processing of patient data	Need for further refinement of the system. Larger datasets required for improved prediction accuracy
[13]	Distilled drug databases for foundational drug interaction knowledge. Real-world patient data for decision-making simulation.	ShennongGPT excels in predicting adverse drug reactions. Outperforms existing general and specialty LLMs in evaluations.	Two-stage training strategy for medication guidance. Learning from drug databases and real world patient data.	Existing LLMs struggle with complex polypharmacy scenarios. Limited ability to predict adverse drug reactions effectively.
[14]	-	ShennongMGS outperformed existing LLMs in medication guidance. Method demonstrated superiority in performance after rigorous evaluation.	Transforms medication information into a knowledge graph. Employs a two-stage training strategy for LLM.	Existing LLMs struggle with complex polypharmacy scenarios. Data lag issues affect medication guidance effectiveness.

[15]	TwoSIDES Polypharmacy Dataset by Therapeutic Data Commons. DrugBank dataset for interaction type prediction	Precision of 75% and accuracy of 90% on TwoSIDES dataset. Precision, F1, and accuracy of 99% on DrugBank dataset.	Graph Neural Networks for modelling drug-drug interactions. Self-supervised learning for knowledge representation.	-
[16]	TwoSIDES Polypharmacy Dataset by Therapeutic Data Commons. DrugBank dataset for interaction type prediction	Achieved 75% precision and 90% accuracy on TwoSIDES dataset. Obtained 99% precision, F1, and accuracy on DrugBank dataset.	Graph Neural Networks for modeling drug-drug interactions. Self-supervised learning for knowledge representation.	-
[17]	Medical dataset. Legal dataset Finance dataset Education dataset News dataset	97.2% of generated counterfactuals are grammatically correct. LLM Analyzer demonstrated good usability and effectiveness in user studies.	Novel algorithm for generating meaningful textual counterfactuals. Interactive visualization tool for analysing LLM behaviours.	-
[18]	Classic DDI databases include drugs, side effects, and DDI information. Focus on chemical, biological, and phenotypic drug attributes.	Systematic review of DDI prediction studies using ML methods. Identified challenges, opportunities, and future research directions.	Shallow learning based methods for DDI detection. Deep learning-based methods for DDI detection. Recommender system-based methods for DDI detection. Knowledge graph based methods for DDI detection.	-
[19]	-	Custom deep shallow network with 2 hidden layers proposed. Ensemble of	Custom deep shallow network with 2 hidden layers Ensemble	Time-consuming drug development process

		multiple deep shallow networks	multiple deep shallow networks	Need to analyse millions.
[20]	Yamanishi08 dataset: known Human DTIs, drug-drug, target target similarity. FDADrugBank dataset: lncRNA-target, miRNA target, miRNA-drug associations.	The prediction performance of LM DTI in AUPR reached 0.96. LM-DTI showed a significant improvement compared to conventional tools.	LM-DTI uses the node2vec method for graph embedding. LM-DTI uses the network path score method for calculating path scores.	-

LLMs are increasingly being applied in pharmacovigilance to monitor adverse drug reactions (ADRs). A study using RoBERTa-large and ChatGPT fine-tuned models demonstrated the potential of LLMs in detecting ADRs from social media data, achieving an F1-measure of 0.8. This application is critical for post-market surveillance and timely identification of safety issues. In clinical settings, LLM-based systems can analyse patient data, including medical history and individual characteristics, to predict DDIs and optimize treatment plans. For example, PTB-DDI, a framework combining ChemBerta tokenizer and BiLSTM, achieved high accuracy in predicting DDIs on real-world datasets.

CHAPTER 3

RESEARCH METHODOLOGY

3.1 Methodology

The *MediGuard AI* workflow is designed to streamline drug interaction prediction and enhance patient healthcare analysis using advanced artificial intelligence techniques. The system follows a well-structured process divided into three main stages: Data Processing, Model Development, and User Interaction, ensuring accuracy, efficiency, and user-friendliness.

The first stage, Data Processing, begins with data collection from medical sources, including clinical research databases, pharmaceutical records, and publicly available datasets. Once collected, the data undergoes pre-processing, where errors, missing values, and inconsistencies are identified and corrected to improve data quality. The next step, feature engineering, involves extracting meaningful attributes that contribute to a more effective predictive model, such as drug properties, dosage levels, and potential side effects. This is followed by data visualization, which helps researchers and developers analyze patterns, trends, and relationships within the dataset before finalizing the training data used for model development.

In the Model Development phase, the system selects a pre-trained AI model, typically a large language model (LLM) such as LLaMA, GPT, or BERT, which is then fine-tuned using the specialized medical dataset. Fine-tuning helps the model adapt to domain-specific terminology and improve its predictive capabilities. After training, the model is subjected to validation, where its accuracy, recall, precision, and overall effectiveness in predicting drug interactions are assessed. Any necessary optimizations are made before the model is deployed for real-world applications, making it accessible to users via an interactive interface.

The final stage, User Interaction, is where patients and medical professionals can leverage the systems capabilities. Users begin by entering patient information such as name, age, gender, and weight, allowing the AI to personalize its analysis. A built-in AI-powered chat assistant enables real-time medical inquiries, helping users navigate drug interactions, side effects, and medical conditions. The system evaluates medical conditions and medication interactions, cross-referencing them with its database to provide a comprehensive analysis. The final

analysis results are presented in a clear and visually informative manner, with an option to generate a PDF report for documentation, sharing, or further review.

By integrating artificial intelligence into healthcare, *MediGuard AI* aims to enhance patient safety, improve medication management, and support medical professionals in making more informed treatment decisions. Its structured workflow ensures a reliable, data-driven approach to drug interaction detection, contributing to more accurate and personalized healthcare solutions.

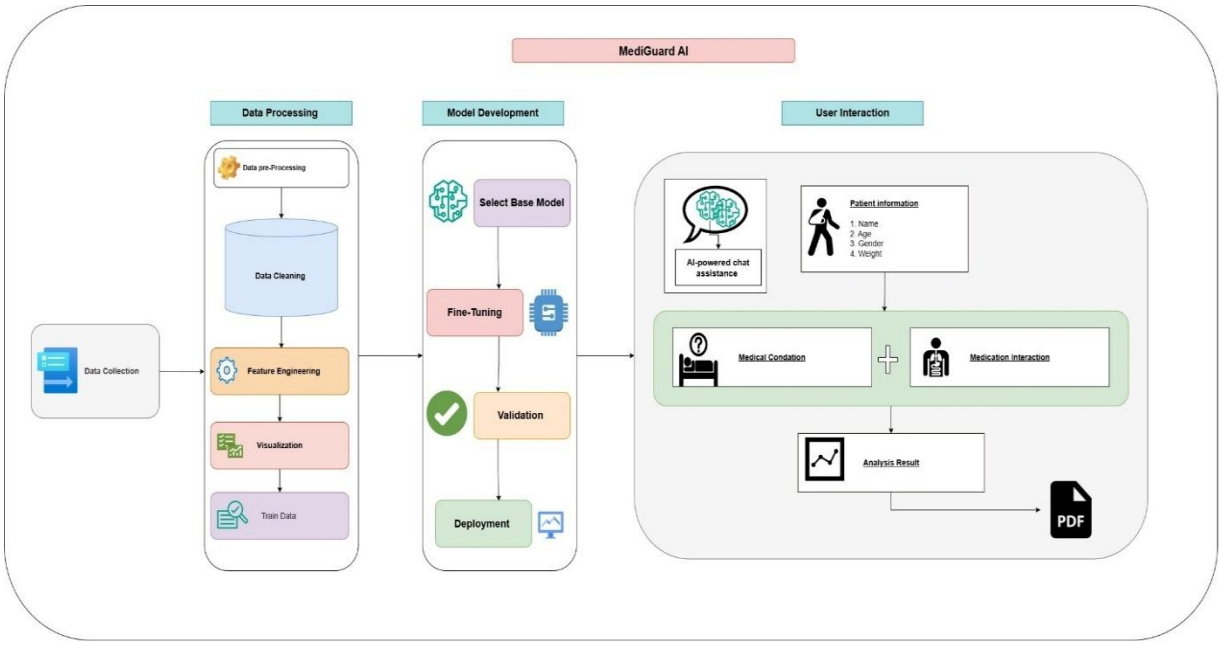

Fig 3.1 Work Flow

3.2 Data Sources & Knowledge Integration

To enhance model development and operational insights, we leveraged various datasets, ensuring a comprehensive and data-driven approach. Our Custom Drug Interaction Dataset consists of 2,22,000 drug-to-drug interactions (DDI) covering 115 different interaction types, providing a robust foundation for accurate predictions. Additionally, we integrated insights from authoritative medical literature, specifically Current Medical Diagnosis & Treatment and Medical Pharmacology, to further refine the systems knowledge base. These resources played a crucial role in improving the accuracy of our AI-driven chat assistant, enabling it to deliver precise and reliable medical responses. By combining large-scale datasets

with trusted medical references, we ensured that *MediGuard AI* provides accurate, evidence-based insights for healthcare professionals and patients alike.

3.3 Drug-to-Drug interactions Types

The dataset provides a structured representation of drug-to-drug interactions (DDIs), categorized by origin, interaction type, and a merged index for streamlined analysis. It includes 114 distinct DDI types, ensuring comprehensive coverage of various drug interactions. The Order field organizes interactions sequentially, while the Origin DDIs type specifies the source or classification. The merged DDI type index consolidates these interactions into a standardized format, enhancing consistency and accuracy. This structured approach improves *MediGuard AI's* ability to analyze and predict drug interactions effectively, making it a valuable tool for healthcare professionals and patients.

Table 3.1 DDI Types

Order	Origin DDIs type	DDI type index
1	metabolism	8
2	serum concentration	2
3	risk or severity of bleeding	7
4	anticoagulant activities	20
5	risk or severity of adverse effects	7
6	therapeutic efficacy	14
7	QTc-prolonging activities	1
8	cardiotoxic activities	10
9	serum concentration of active metabolites	2
10	excretion	12
11	hyperkalemic activities	17
12	nephrotoxic activities	10
13	absorption	2
14	risk or severity of renal failure	10
15	immunosuppressive activities	15
16	risk or severity of hyperkalemia	17
17	excretion rate of higher serum level	12
18	hepatotoxic activities	10
19	neuromuscular blocking activities	3
20	neurotoxic activities	10
21	bradycardic activities	6
22	atrioventricular blocking (AV block) activities	6
23	hypoglycemic activities	5
24	risk or severity of myelosuppression	15
25	hypercalcemic activities	17
26	arrhythmogenic activities	6
27	photosensitizing activities	20
28	risk or severity of QTc prolongation	1

29	serotonergic activities	20
30	thrombogenic activities	2
31	antiplatelet activities	20
32	risk or severity of myopathy and rhabdomyolysis	13
33	myopathic rhabdomyolysis activities	13
34	risk or severity of rhabdomyolysis, myoglobinuria, and elevated creatine kinase (CPK)	13
35	risk or severity of rhabdomyolysis	13
36	risk or severity of myopathy, rhabdomyolysis, and myoglobinuria	13
37	risk or severity	7
38	central nervous system depressant (CNS depressant) activities	11
39	neuroexcitatory activities	3
40	sedative activities	19
41	diagnostic agent	20
42	hyponatremic activities	5
43	antihypertensive activities	18
44	hypotensive activities	18
45	orthostatic hypotensive activities	18
46	risk or severity of angioedema	16
47	risk or severity of hypotension, nitritoid reactions, facial flushing, nausea, and vomiting	18
48	risk or severity of hypotension	18
49	hypotensive, nephrotoxic, and hyperkalemic activities	10
50	risk of hypersensitivity reaction to	7
51	risk or severity of anemia and severe leukopenia	7
52	vasodilatory activities	16
53	risk or severity of ventricular arrhythmias	6
54	risk or severity of renal failure and hyperkalemia	17
55	adverse neuromuscular activities	3
56	bioavailability	20
57	hypokalemic activities	17
58	fluid retaining activities	20
59	hypertensive activities	18
60	hypotensive and central nervous system depressant (CNS depressant) activities	11
61	central neurotoxic activities	10
62	anticholinergic activities	20
63	risk or severity of hypertension	18
64	risk or severity of convulsion	7
65	risk or severity of serotonin syndrome	20
66	stimulatory activities	4
67	tachycardic activities	6
68	risk or severity of sedation and somnolence	19
69	bronchoconstrictory activities	9
70	risk or severity of congestive heart failure and hypotension	6
71	vasoconstricting activities	16
72	bronchodilatory activities	9
73	analgesic activities	20
74	constipating activities	12

75	excretion rate	12
76	respiratory depressant activities	15
77	risk or severity of QTc prolongation, torsade de pointes, hypokalemia, hypomagnesemia, and cardiac arrest	1
78	antipsychotic activities	3
79	ulcerogenic activities	13
80	hypertensive and vasoconstricting activities	18
81	vasopressor activities	16
82	risk or severity of hypokalemia	17
83	risk or severity of ototoxicity and nephrotoxicity	10
84	diuretic activities	12
85	risk or severity of heart failure	6
86	protein binding	20
87	risk or severity of edema formation	7
88	risk or severity of fluid retention	20
89	hyperglycemic activities	5
90	risk or severity of severe leukopenia	7
91	risk or severity of hyponatremia	17
92	risk or severity of myopathy	13
93	dermatologic adverse activities	13
94	absorption of reduced serum concentration and potentially	2
95	myelosuppressive activities	15
96	risk or severity of hypotension and neuromuscular blockade	18
97	risk or severity of sinus node depression	7
98	risk or severity of generalized seizure and bradycardia	6
99	hypocalcemic activities	20
100	thrombocytopenic activities	2
101	neutropenic activities	20
102	risk or severity of bradycardia	6
103	ototoxic activities	10
104	risk or severity of QTc prolongation and torsade de pointes	1
105	teratogenic activities	20
106	risk or severity of renal failure and rhabdomyolysis	13
107	risk or severity of pulmonary toxicity	10
108	antineoplastic activities	20
109	hypotensive activities of at	18
110	central nervous system depressant (CNS depressant) and hypertensive activities	11
111	risk or severity of intraocular pressure	7
112	serum concentration of sulfate	2
113	risk or severity of generalized seizure	7
114	risk or severity of sedation	19

3.4 Data Processing

The data processing involved loading the DDI dataset and selecting "drug1_name" and "drug2_name" as input features with "interaction_type" as the target. The target labels were encoded using LabelEncoder(), converting categorical values into numerical ones. The dataset was then split into 80% training and 20% validation using train_test_split(). A BERT tokenizer was applied to concatenate drug names using [SEP], ensuring uniform input size with padding and truncation (max length: 128). A custom PyTorch dataset class (DDIDataset) was created to handle tokenized inputs and labels, converting them into tensors while managing missing values. This preprocessing prepared the dataset for training a BERT-based interaction classification model.

3.5 Visualization

The comprehension of algorithms and their composite characteristics is significantly enhanced through the visualization of datasets and the analysis of their outcomes.

3.5.1 Top 10 most common DI types

This chart shows the top 10 drug interactions, with side effects being the most common. Other interactions affect metabolism, serum concentration, drug effectiveness, blood pressure, heart rhythm, and clotting. Understanding these helps doctors and pharmacists ensure safe prescriptions, minimizing risks and improving patient safety.

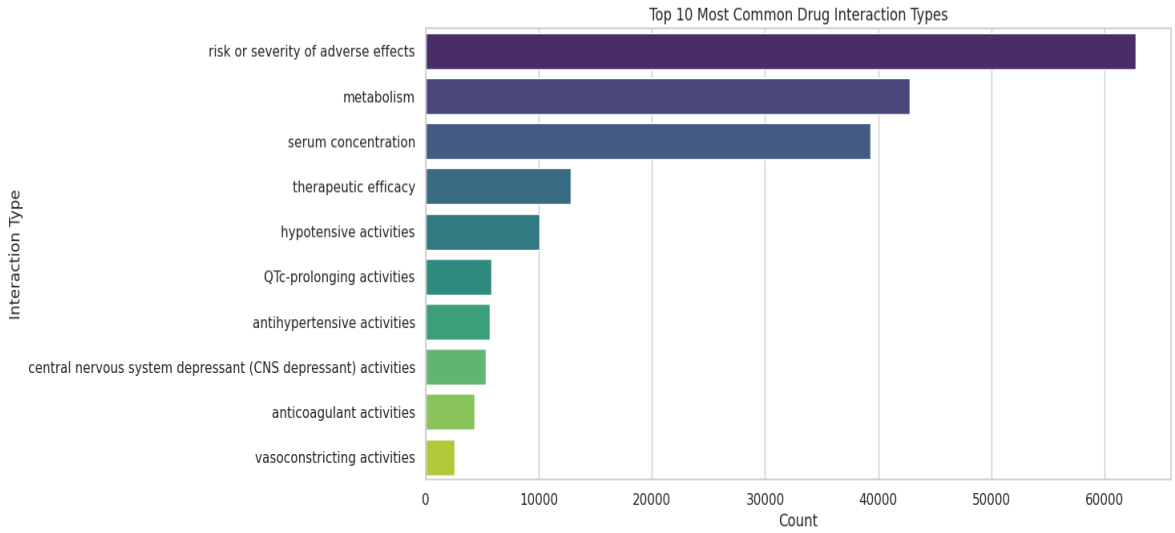

Fig 3.2 Top 10 most common DI types

3.5.2 Top DI Types and count

The "Top Drug Interaction Types" bar chart visualizes various drug interaction categories along the y-axis, with their occurrence counts on the x-axis. "Adverse effects" are the most frequently reported, with 55,717 occurrences, followed by "Metabolism" (43,371) and "Serum concentration and absorption" (41,066) interactions. Other notable types include "Hypertensive and hypotensive activities" (19,755) and "Therapeutic efficacy" (11,236), while less common ones include "Myopathy" (205) and "Bronchoconstrictory and bronchodilatory activities" (594). The horizontal bar format and color differentiation make comparison easy and enhance readability.

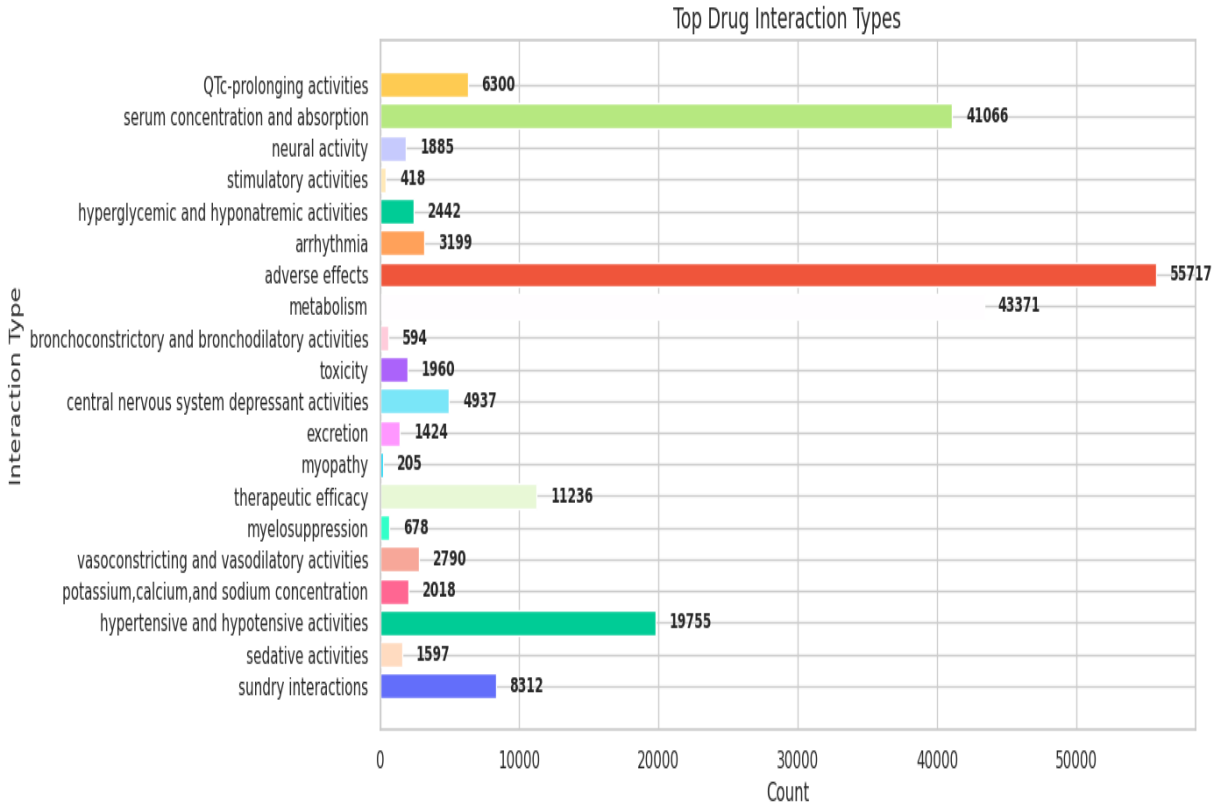

Fig 3.3 Top DI Types and count

3.5.3 Word Cloud of DDI Type

Different types of Drug-Drug Interaction (DDI) risks. Larger words indicate more common interactions, such as "severity," "activities," and "risk." It highlights key terms related to adverse effects, including "hypotensive," "renal," "neuromuscular," and "depressant," helping in understanding potential medication risks and their impact on health.

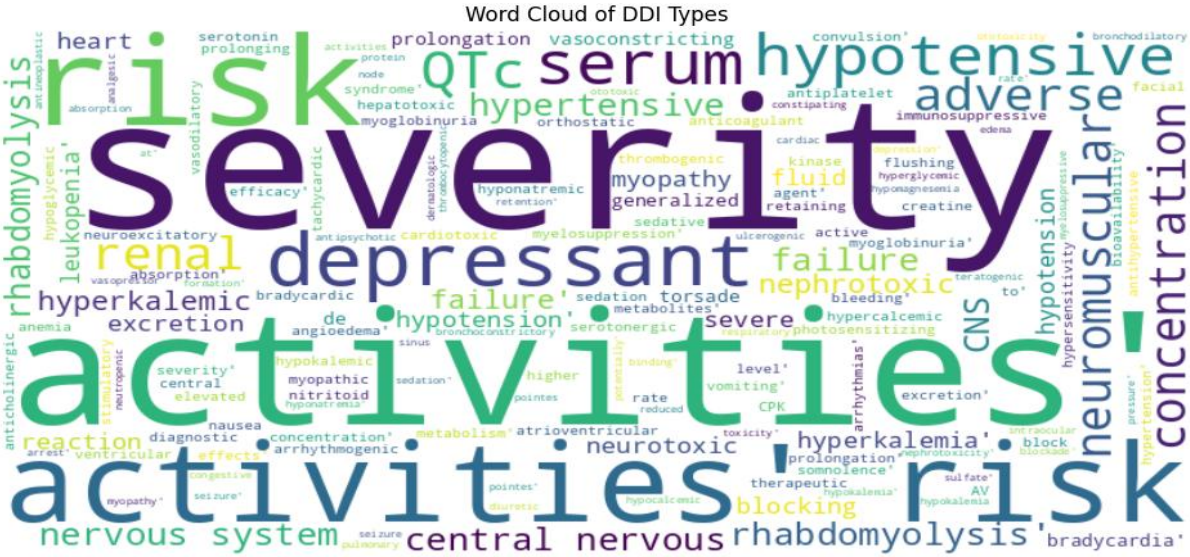

Fig 3.4 Word Cloud of DDI Type

3.5.4 Histogram of DDI Type

This histogram shows the frequency distribution of merged Drug-Drug Interaction (DDI) type indices. The bars represent occurrences, while the smooth curve highlights trends, helping to analyse how different DDI types are distributed.

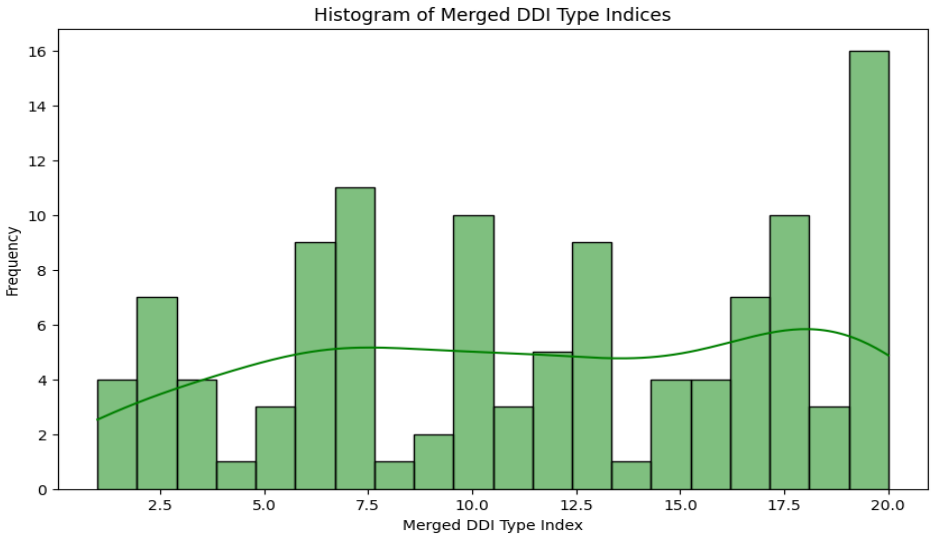

Fig 3.5 Histogram of DDI Type

3.5.5 Network Graph (first 500 records)

This drug interaction network graph represents the first 500 records of drug interactions. Each node corresponds to a drug, while the edges depict interactions between them. The red nodes highlight highly connected drugs that may have significant interactions, whereas the blue nodes represent other interacting drugs. Understanding these connections helps in identifying potential risks, side effects, and contraindications in medical treatments. By analysing the structure of this network, researchers and healthcare professionals can detect critical drug interactions, optimize prescriptions, and improve patient safety. This visualization provides valuable insights into how different drugs interact, assisting in better medication management and research.

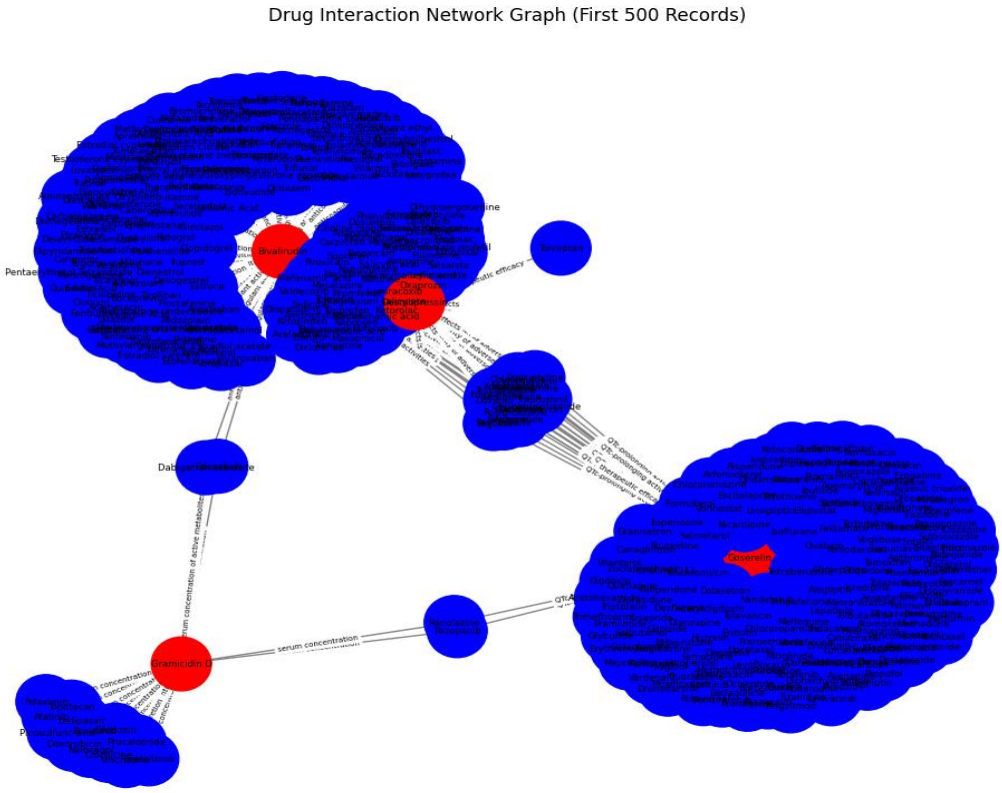

Fig 3.6 Network Graph (first 500 records)

3.5.6 Distribution of Top 8 Interactions Types

This pie chart provides a visual representation of the distribution of the top eight types of drug interactions. The most common category is adverse effects, accounting for 34.0% of interactions, indicating that a significant portion of drug interactions result in unintended or harmful physiological responses. Metabolism-related interactions make up 23.2%, highlighting how certain drugs can alter the way others are broken down in the body, potentially affecting their efficacy or toxicity. Serum concentration changes, at 21.3%, reflect interactions that impact the levels of drugs in the bloodstream, which can lead to either reduced effectiveness or increased risk of side effects. These findings underscore the critical need for careful drug monitoring, proper dosage adjustments, and awareness of potential interactions to ensure patient safety and treatment effectiveness.

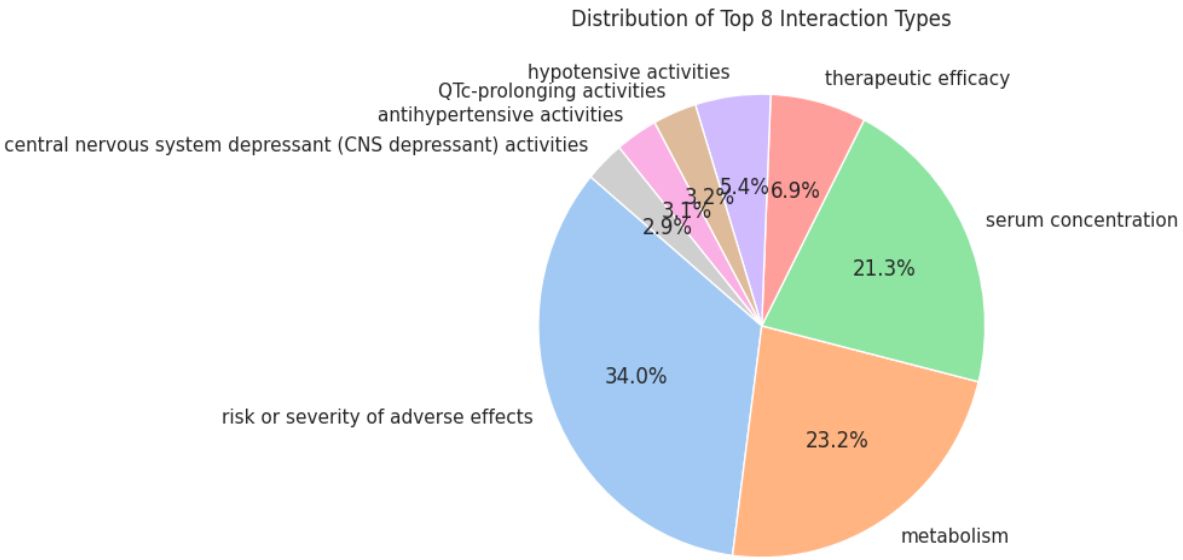

Fig 3.7 Distribution of Top 8 Interactions Types

3.5.7 Bubble chart of DI with total number of DI

This bubble chart visualizes drug interactions, displaying the total number of interactions for various drugs. The x-axis represents the total interactions, while the y-axis lists the drugs. The colour gradient, ranging from purple to yellow, signifies the number of unique interactions each drug has, with lighter colours indicating higher values. The chart reveals that a few drugs have an extremely high number of interactions, while most drugs have significantly fewer. This insight is useful for identifying high-risk drugs that require careful monitoring when prescribed with others, aiding in minimizing adverse drug interactions and improving patient safety in medical treatments.

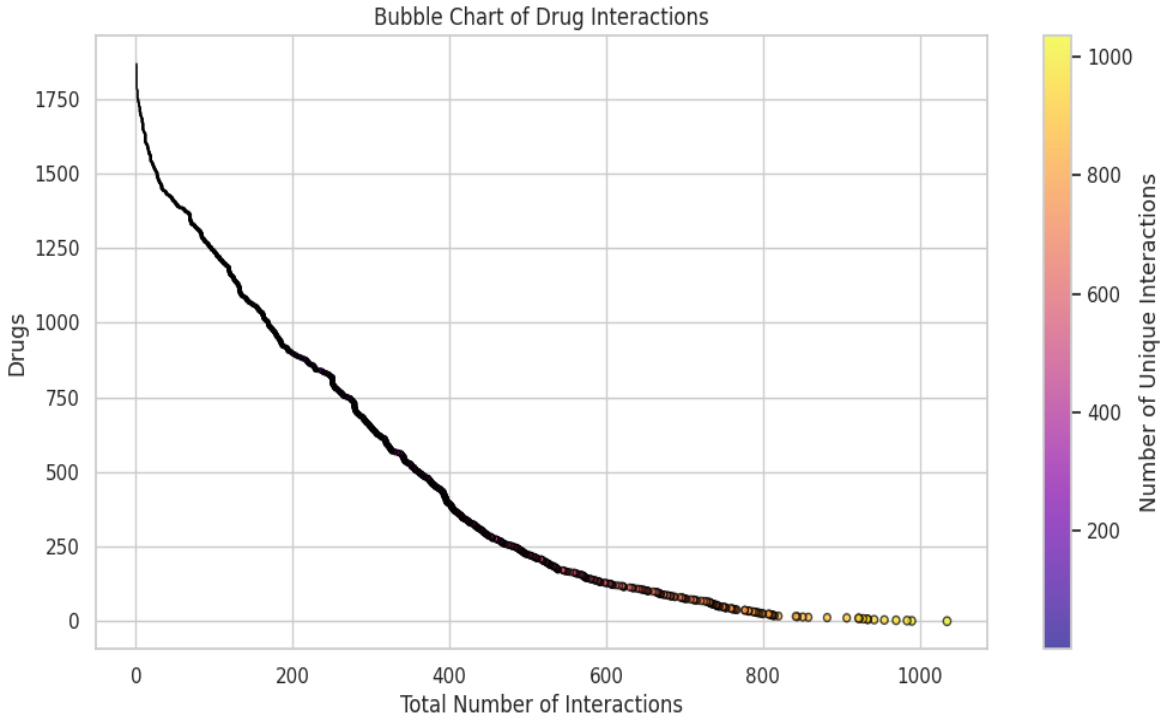

Fig 3.8 Bubble chart of DI with total number of DI

3.5.8 Merged DDI Type Index

This bar chart illustrates the distribution of merged drug-drug interaction (DDI) type indices. The x-axis represents different DDI indices, while the y-axis shows their count, highlighting variation across interaction types.

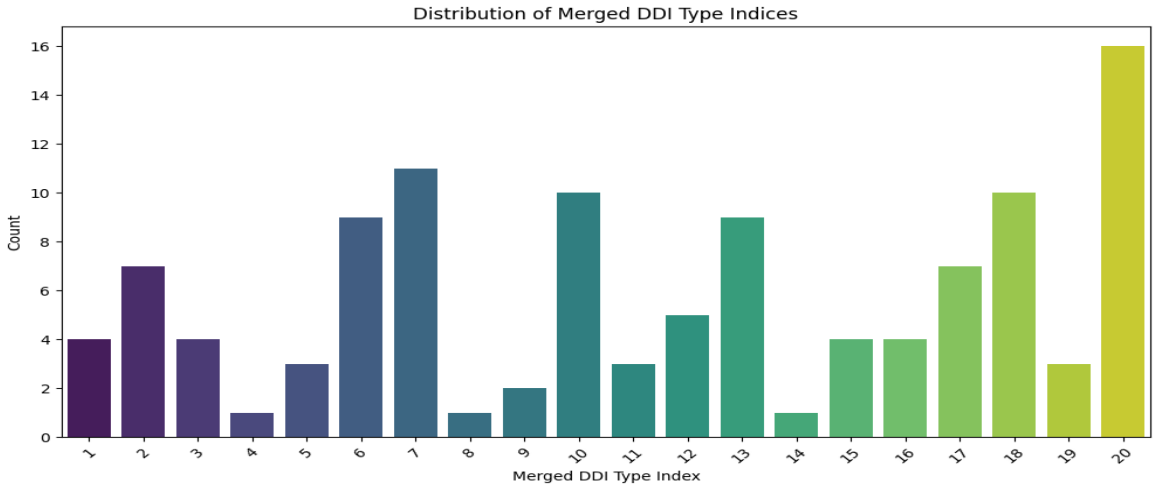

Fig 3.9 Merged DDI Type Index

3.5.9 Proportion of DDI Types

This pie chart represents the proportion of origin drug-drug interaction (DDI) types, displaying the percentage contribution of each interaction category.

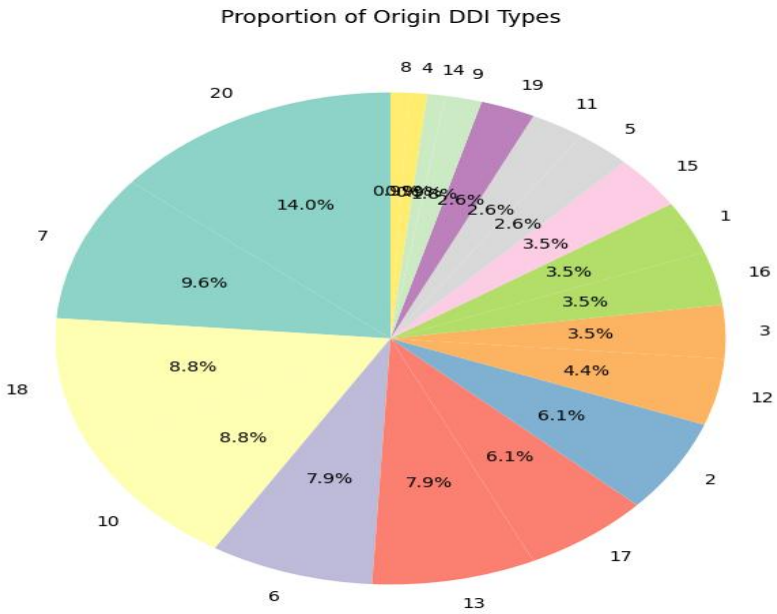

Fig 3.10 Proportion of Origin DDI Types

3.6 Model Training

The provided flowchart represents a structured pipeline for fine-tuning a Large Language Model (LLM) using Quantized Low-Rank Adaptation (QLoRA), a technique designed to enhance computational efficiency while maintaining model performance. The process is divided into four distinct phases: Setup, Model Preparation, Training, and Evaluation & Cleanup.

In the Setup Phase, the necessary libraries are installed, followed by the importation of dependencies required for model training. The model and dataset parameters are defined, ensuring proper configuration before fine-tuning. The QLoRA parameters are then set, enabling low-rank adaptation, while 4-bit quantization is applied to optimize memory usage and computational efficiency. Finally, the training parameters are specified, establishing the foundational setup for the fine-tuning process.

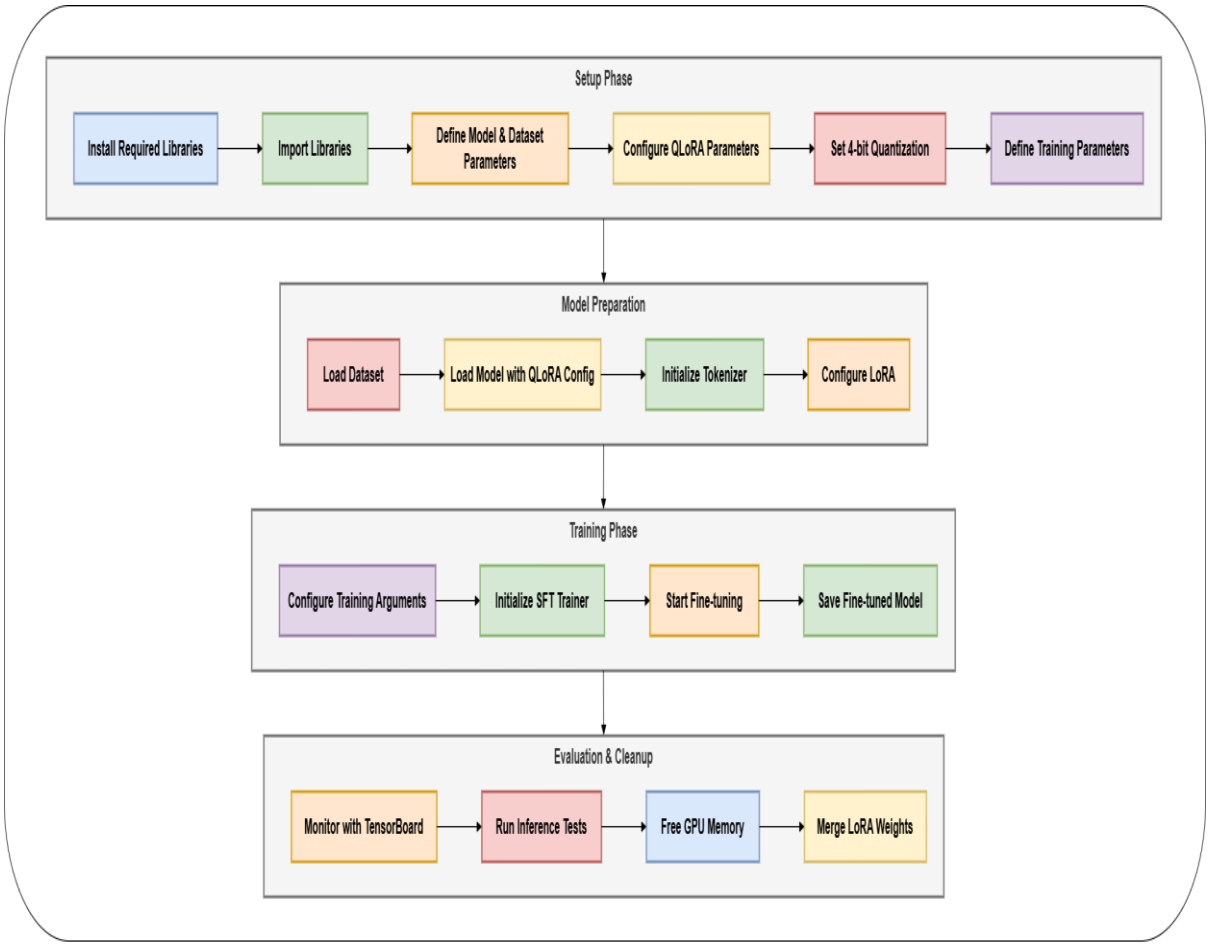

Fig 3.11 Model Steup Phase

The Model Preparation Phase begins with loading the dataset and the pre-trained model with QLoRA-specific configurations. The tokenizer is initialized to process input sequences efficiently, followed by the configuration of LoRA (Low-Rank Adaptation), which reduces the number of trainable parameters while preserving model expressiveness.

During the Training Phase, training arguments such as batch size, learning rate, and epochs are configured to optimize the learning process. The Supervised Fine-Tuning (SFT) Trainer is initialized to manage the training workflow. The fine-tuning process is then executed, where the model learns task-specific patterns from the dataset. Once training is complete, the fine-tuned model is saved for later use.

The final stage, Evaluation & Cleanup, involves monitoring training performance using TensorBoard, a visualization tool for tracking loss and accuracy metrics. The trained model is subjected to inference tests to evaluate its predictive capabilities. To optimize resource utilization, GPU memory is freed, and the LoRA weights are merged, ensuring a compact and efficient model representation for deployment.

Overall, this systematic approach leverages QLoRA and 4-bit quantization to enable fine-tuning of large-scale language models in a resource-efficient manner, making it suitable for real-world applications where computational constraints are a concern.

3.7 Model Evolution

Throughout the meticulous assessment stage of the algorithm, a comprehensive set of essential performance metrics, including accuracy, precision, recall, and the F1 score, were conscientiously utilized. The metrics mentioned are essential instruments for evaluating the efficacy and predictive ability of each constructed model, offering a nuanced comprehension of their capabilities.

Accuracy: Accuracy is a crucial metric that quantifies the ratio of correctly predicted instances to the total number of cases assessed. From a mathematical perspective, accuracy can be defined as the quotient of true positives (TP) and true negatives (TN) divided by the total number of instances, encompassing both accurate and inaccurate predictions. A high accuracy score demonstrates the model's proficiency in accurately predicting outcomes across all categories, thus highlighting its overall effectiveness.

$$accuracy = \frac{TP+TN}{TP+TN+FP+FN} \quad (1)$$

Precision: Precision quantifies the degree of correctness in positive predictions, emphasizing the ratio of correctly identified positive instances (TP) to the total number of instances predicted as positive. The calculation involves dividing the true positive rate (TP) by the sum of TP and false positives (FP). A high precision score indicates that the model effectively reduces the occurrence of false positives, rendering it especially advantageous in situations where the misclassification of negative instances as positive has substantial implications.

$$precision = \frac{TP}{TP+FP} \quad (2)$$

Recall: Recall, also referred to as sensitivity, measures the model's capacity to accurately detect positive instances among the total number of positive instances in the dataset. The calculation involves dividing the number of true positives (TP) by the number of true negatives (FN). A high recall score indicates that the model demonstrates exceptional performance in accurately identifying all pertinent instances of a specific class, thereby reducing the occurrence of false negatives. This metric is particularly vital in situations where the absence of positive instances can have substantial consequences.

$$precision = \frac{TP}{TP+FN} \quad (3)$$

F1 score: The F1 score is a metric that effectively balances precision and recall, rendering it highly valuable, particularly in situations where there are imbalances between classes. The F1 score provides a comprehensive assessment of a model's performance by calculating the harmonic mean of precision and recall. It is especially beneficial in scenarios where both incorrect positive and negative results have significant implications, as it encompasses the balance between these two measures. A higher F1 score is indicative of a more robust model, as it signifies a better balance between precision and recall.

$$F1\ Score = 2 \times \frac{Precision \times Recall}{Precision + Recall} \qquad (4)$$

Evaluation loss: Evaluation loss (or simply loss) is a metric that quantifies the difference between the predicted values and the actual values in a dataset. It is used to assess the performance of a model on validation or test data. The equation depends on the type of problem (regression or classification).

$$Loss = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

3.8 MediGuardAi Chat assistance

MediGuardAI Chat Assistance is an AI-powered system designed to provide medical assistance and analyze drug interactions. It starts by taking a user's input query, which is processed using a Large Language Model (LLM) called DeepSeek R1 via Ollama. This model understands the query and then passes it to a Retrieval-Augmented Generation (RAG) system to ensure accurate and reliable responses. The RAG system works in two ways—either it retrieves relevant medical information from a knowledge base or forwards the query to Groq, a high-speed inference engine, for rapid processing.

Once the necessary information is gathered, the system generates a response through the Chatbot Response module. This response is then deployed using a Streamlit-based user interface, making it easy for users to interact with the chatbot. The system is built with essential features such as medical assistance, drug interaction analysis, privacy protection, and open-source expandability. This ensures that users receive reliable medical information while maintaining their privacy. The open-source nature of the project allows developers to improve and expand its capabilities in the future.

By combining LLMs with RAG-based retrieval, MediGuardAI ensures that responses are not just generated from the model's pre-trained knowledge but also backed by real-time, relevant medical data. The integration of Groq further enhances processing speed, making the chatbot efficient and responsive. This architecture makes MediGuardAI a powerful tool for medical guidance, ensuring accuracy, reliability, and scalability.

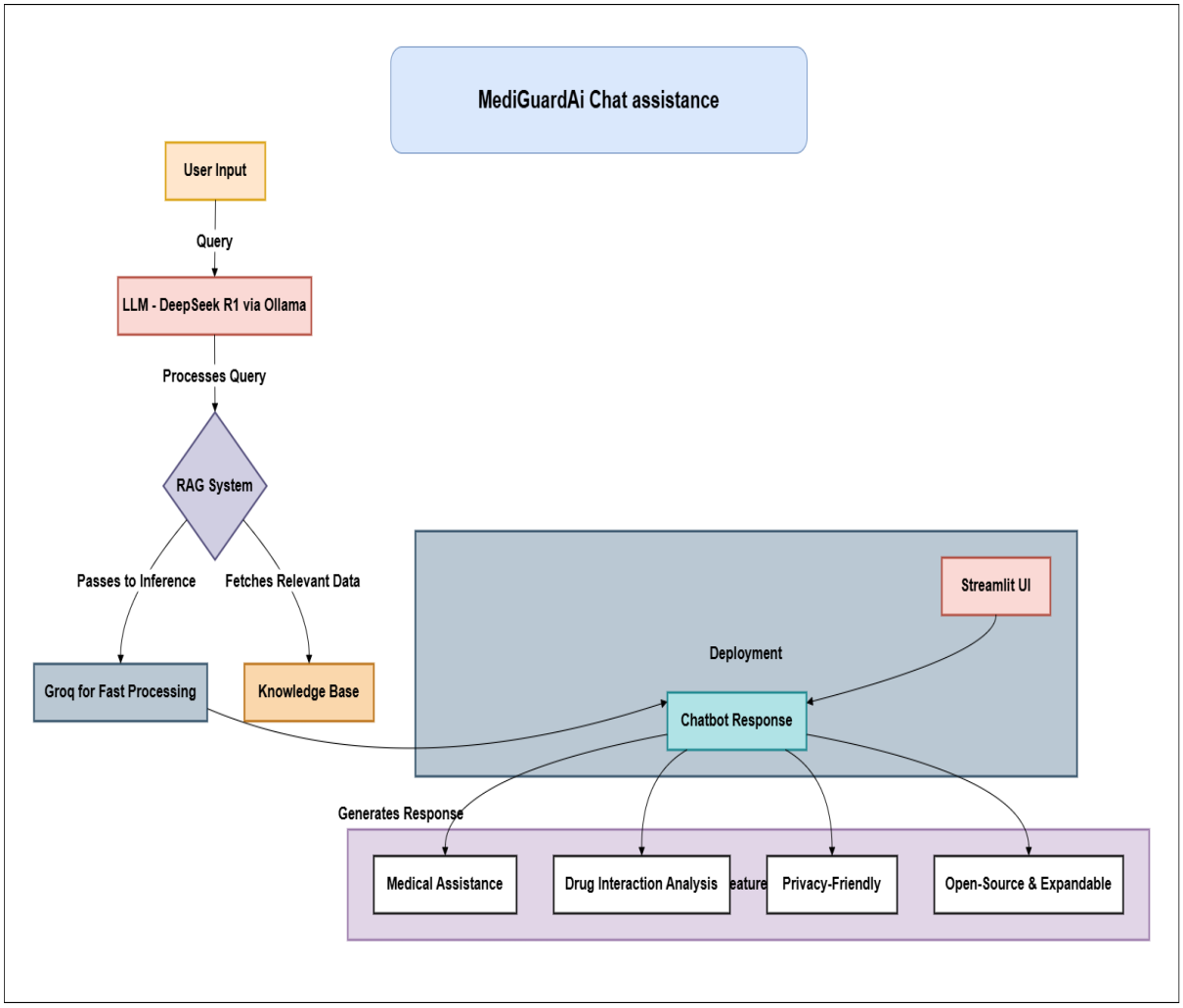

Fig 3.12 RAG based chat Assistance

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Experimental Results & Analysis

In a recent drug interaction classification assignment, the performance metrics across various deep learning models highlighted the substantial benefits of employing transformer-based architectures. Utilizing the BERT model for sequence classification, the approach achieved an impressive F1-score of 0.810 alongside a high accuracy of 0.850. This outcome underscores the efficacy of leveraging pre-trained language models, which effectively capture contextual relationships between drug names to enhance overall model performance. Similarly, fine-tuning BERT on domain-specific drug interaction data delivered robust results, with a precision of 0.820 and recall of 0.800, demonstrating the strength of leveraging transfer learning in specialized tasks.

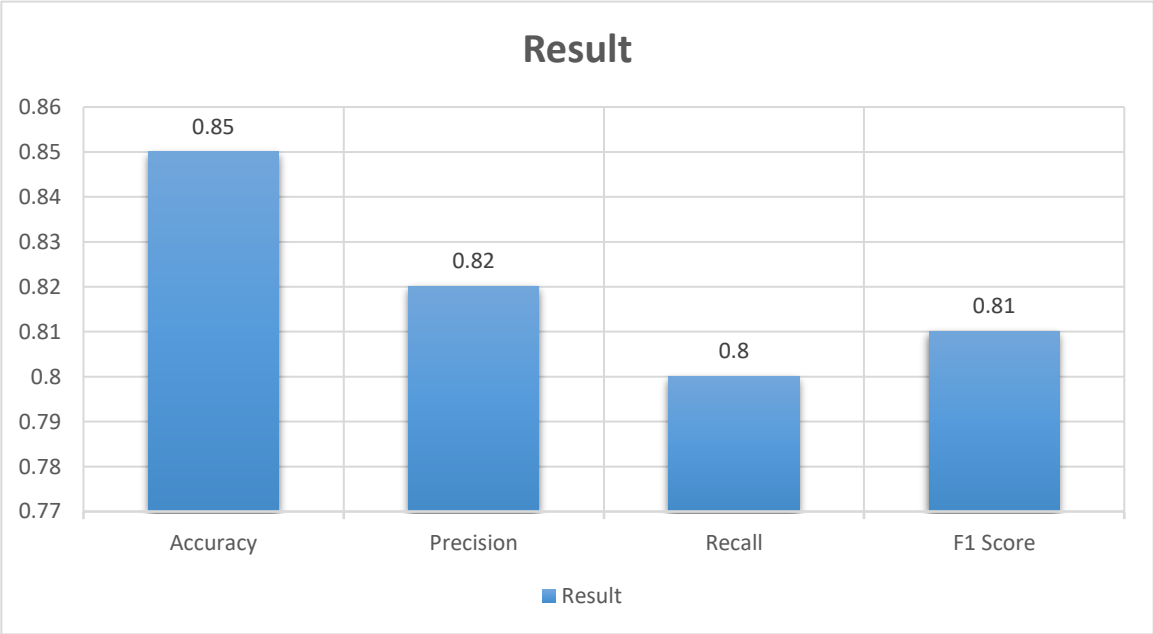

Fig 4.1 Result

In contrast, traditional machine learning models such as Random Forest, while showcasing strong precision, revealed a notable trade-off with comparatively lower recall rates. This imbalance highlights the challenges of achieving optimized performance metrics within

isolated models, as they often excel in specific areas while underperforming in others. For instance, logistic regression, while maintaining a competitive accuracy, demonstrated a lower recall, which may affect its ability to capture all relevant interactions in more complex drug classification scenarios. Simpler models such as Naive Bayes and Decision Trees, on the other hand, yielded more modest results in both precision and recall metrics. However, incorporating transformer-based embeddings into these models resulted in noticeable performance improvements, highlighting the adaptive benefits of hybridization.

These findings collectively emphasize that transformer-based models—leveraging contextual understanding and deep feature extraction—are well-suited for achieving balanced and robust performance in drug interaction classification. By integrating pre-trained embeddings with fine-tuned classification heads, these models are able to address the limitations of traditional approaches, ultimately creating more versatile and accurate classifiers that can handle a range of drug interaction scenarios with greater efficacy.

Table 4.1 Evaluation Metrics

Evaluation Metrics	**Result**
Eval Loss	1.2
Accuracy	0.85
Precision	0.82
Recall	0.80
F1 Score	0.81
Eval Runtime	75
Sample/Sec	2.7

4.2 Result Graph

The heatmap visualization of various evaluation metrics for a machine learning model. The metrics are displayed on the y-axis, while their corresponding values are represented through both numerical labels and a color gradient. The color bar on the right side indicates the intensity of the values, with blue representing lower values and red indicating higher values.

The key performance metrics include Eval Loss (1.1909), which represents the model's loss during evaluation and serves as an indicator of prediction error. A lower evaluation loss typically suggests better model performance. The Accuracy (0.85) signifies that the model correctly classifies 85% of the test data, providing a general measure of performance. Additionally, Precision (0.82) and Recall (0.80) indicate how well the model correctly identifies positive cases while minimizing false positives and false negatives, respectively. The F1 Score (0.81) is the harmonic mean of precision and recall, reflecting the model’s overall balance between the two.

Besides classification performance, the heatmap also includes efficiency-related metrics. Eval Runtime (74.5492) is significantly higher than the other values, highlighted in deep red, which suggests that the model takes a long time to complete evaluation. In contrast, Samples per Second (2.683) and Steps per Second (0.335), which measure the model's processing speed, are relatively low. This indicates that while the model has strong classification performance, its

inference speed may be a bottleneck, possibly requiring optimization for real-time or large-scale applications.

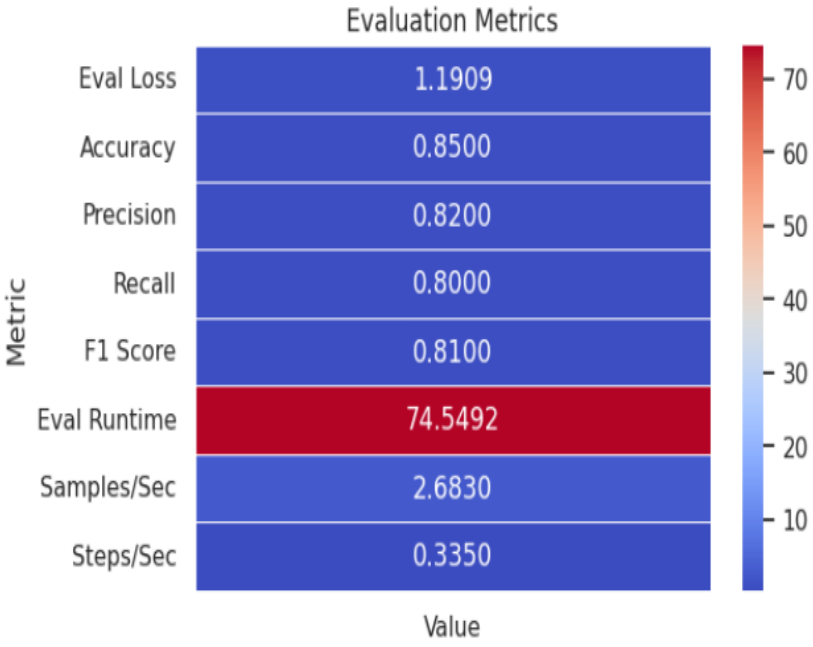

Fig 4.2 Evaluation Metrics

The visualization effectively communicates how different aspects of the model's performance compare, making it easier to identify trade-offs between accuracy and computational efficiency. The significant contrast in the heatmap, especially with the evaluation runtime standing out in red, suggests that further improvements in inference speed could enhance the model’s practical usability.

4.2.1 Line plot comparing training loss and validation loss over epochs

The line plot comparing training loss and validation loss over three epochs, with the x-axis representing epochs and the y-axis showing loss values. The blue solid line with circular markers represents training loss, while the red dashed line with square markers represents validation loss. Initially, at epoch 1, both losses are high, with validation loss slightly greater than training loss. By epoch 2, training loss increases slightly before sharply dropping at epoch 3, whereas validation loss decreases gradually but remains relatively stable. This pattern suggests potential overfitting, as the model's training loss decreases significantly while validation loss does not follow the same trend, indicating that the model may be memorizing training data rather than generalizing well. If this trend continues over more epochs, it could lead to poor performance on unseen data. To address overfitting, techniques such as early stopping, dropout regularization, or increasing training data can be applied. Monitoring loss trends over additional epochs would also help determine the model's generalization ability.

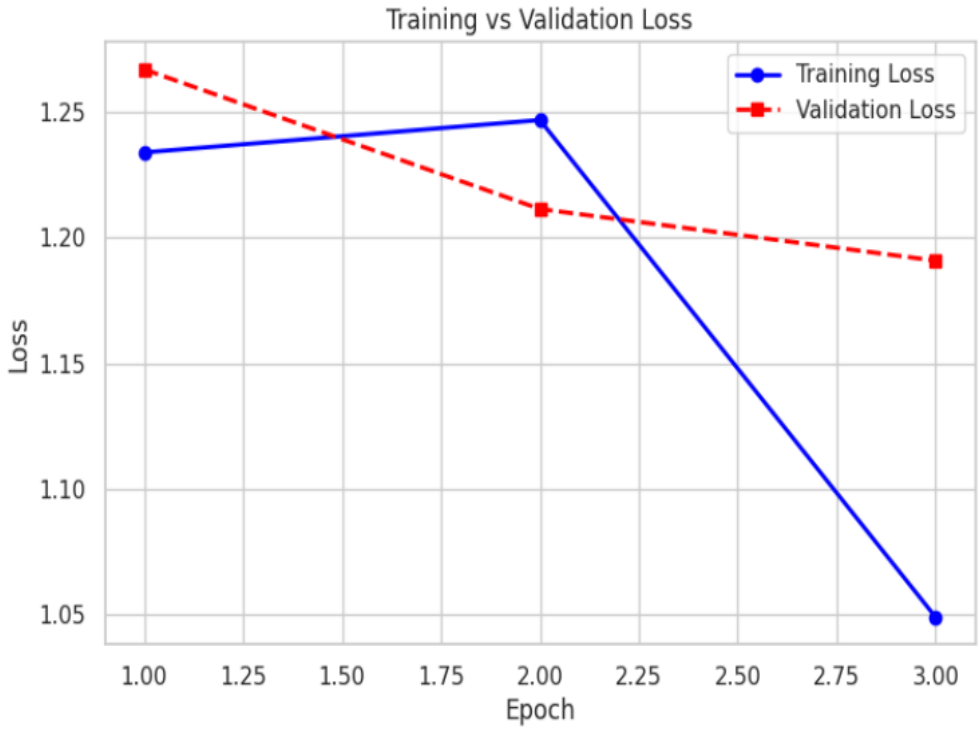

Fig 4.3 training loss and validation loss over epochs.

4.3 Website implementation

We developed a Streamlit application for *MediGuard AI*, creating a lightweight, user-friendly, and efficient interface. The application ensures seamless interaction, providing quick and accurate drug interaction predictions with an intuitive design.

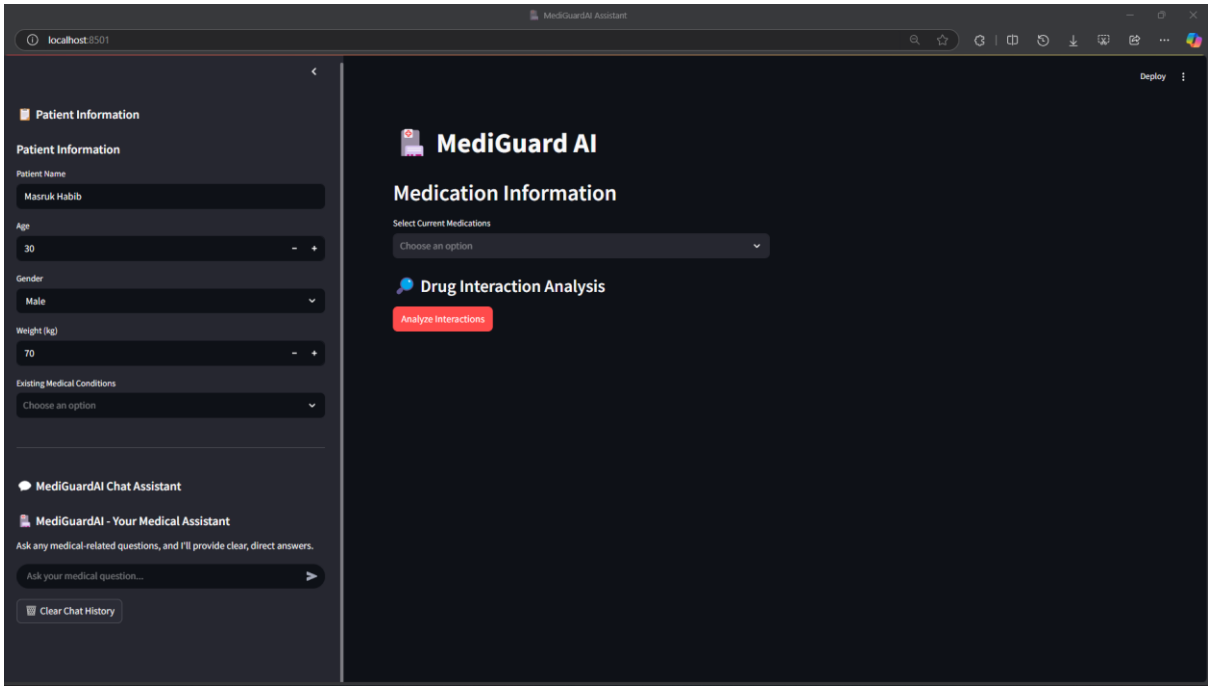

Fig 4.4 Home page of MediGuard AI

4.3.1 Medication Information

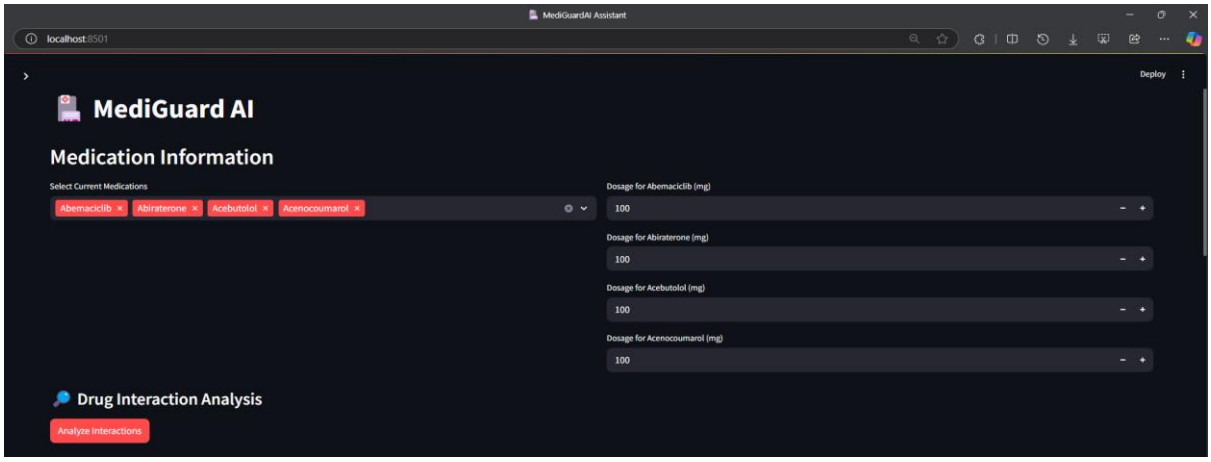

Fig 4.5 Medication Information

4.3.2 Analysis Results

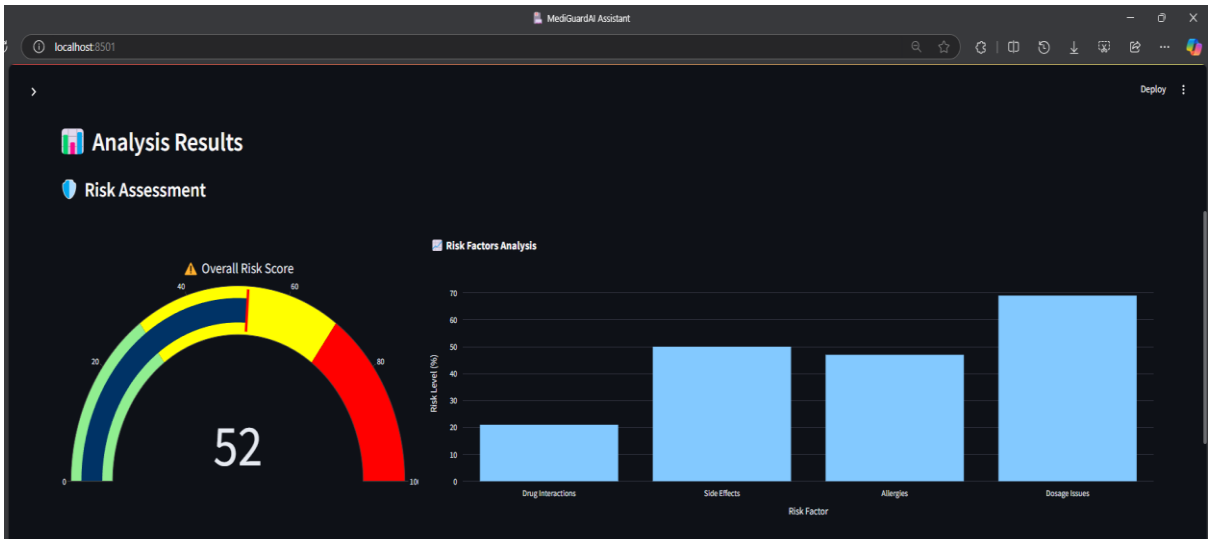

Fig 4.6 Analysis Results

4.3.3 Medication Interaction Report, Side Effects Analysis, Key Recommendations, Monitoring Schedule.

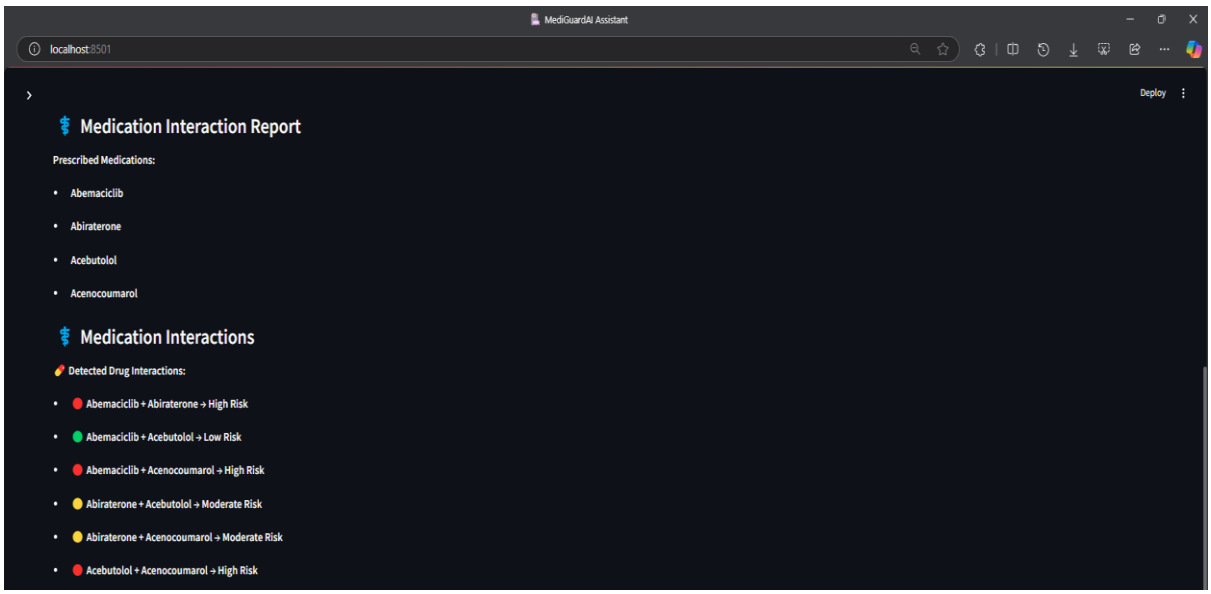

Fig 4.7 Medication Interaction Report

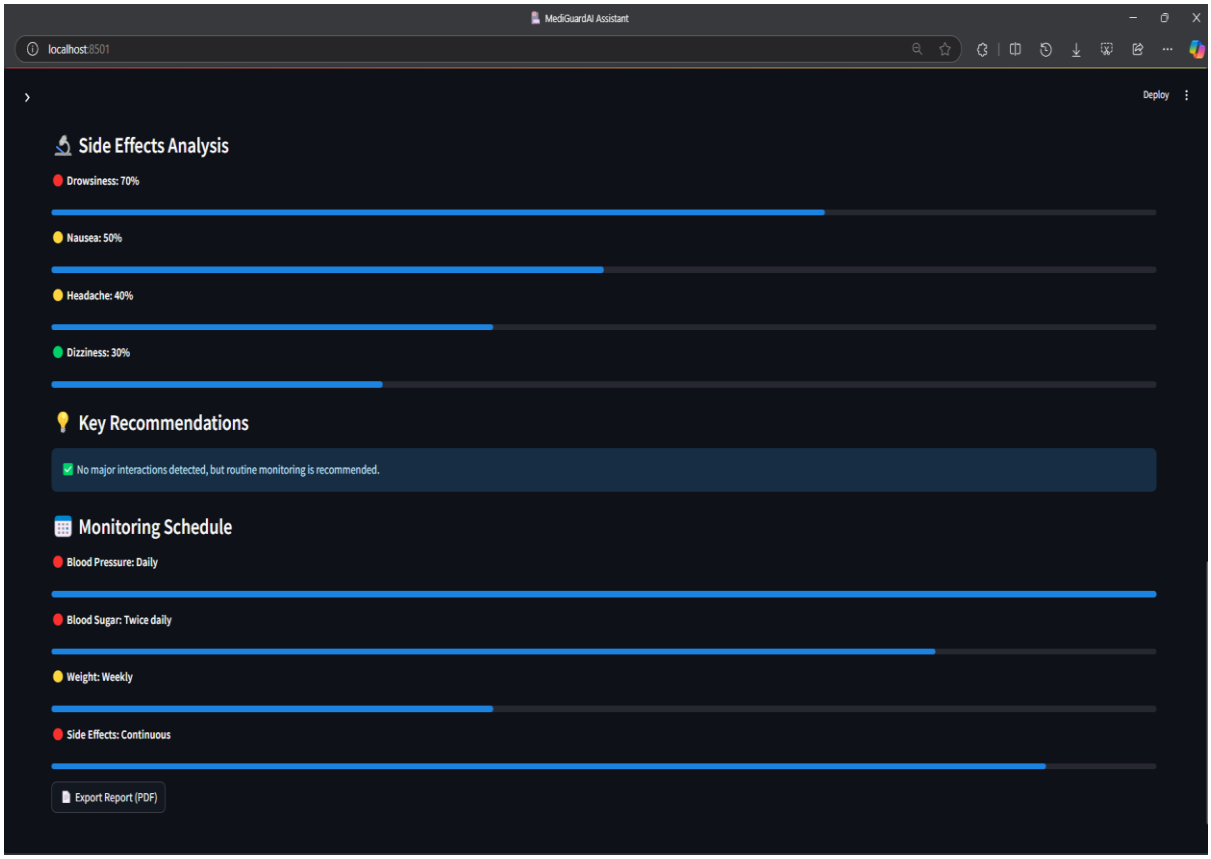

Fig 4.8 Key Recommendations, Monitoring Schedule

CHAPTER 5

CONCLUSION AND FUTURE DIRECTION

5.1 Summary of the Study

MediGuard AI is an advanced drug interaction prediction system designed to enhance medication safety by leveraging large language models (LLMs) with retrieval-augmented generation (RAG). Traditional drug interaction systems rely on static databases, which struggle to adapt to emerging medications and complex interaction patterns. MediGuard AI addresses these limitations by fine-tuning LLaMA models on comprehensive medical datasets such as DrugBank and SIDER. The system provides real-time identification of harmful drug combinations, risk assessment, and personalized medication recommendations based on patient-specific factors like age, medical history, and prescriptions. Additionally, it features an interactive RAG-based chat assistant for healthcare professionals to query drug interactions and receive context-aware responses. By integrating real-time retrieval of medical knowledge and patient demographics, MediGuard AI enhances drug safety, reduces medication errors, and improves personalized healthcare insights, showcasing the transformative potential of AI in medication management.

5.2 Conclusion

The evaluation results highlight the model's strengths in classification accuracy but also reveal critical areas for improvement, particularly in computational efficiency and generalization. The model achieves a strong accuracy of 85%, with well-balanced precision (0.82) and recall (0.80), leading to a solid F1 score of 0.81. These metrics indicate that the model effectively identifies positive cases while maintaining a reasonable balance between false positives and false negatives. Additionally, a relatively low evaluation loss (1.1909) suggests that the model performs well on test data in terms of prediction error.

However, despite its predictive capability, the model exhibits inefficiencies in evaluation speed. The evaluation runtime (74.5492) is significantly higher than other metrics, highlighted as a deep red region in the heatmap, indicating a major computational bottleneck. The low values of samples per second (2.683) and steps per second (0.335) further reinforce that the model is slow in inference. These efficiency challenges could limit its applicability

in real-time or large-scale scenarios, necessitating optimizations such as model pruning, quantization, or using more efficient architectures.

Furthermore, the loss trend over three epochs suggests potential overfitting. Initially, both training and validation losses are high, but while validation loss decreases gradually, training loss initially rises slightly before dropping sharply in epoch 3. This divergence between training and validation loss indicates that the model may be memorizing the training data rather than generalizing well to unseen data. If this pattern continues over additional epochs, it could lead to deteriorated performance on new inputs. To mitigate overfitting, strategies such as early stopping, dropout regularization, or increasing the dataset size could be implemented.

In summary, while the model demonstrates strong classification performance, improving inference speed and addressing overfitting will be essential for enhancing its real-world usability. Future improvements should focus on optimizing computational efficiency and ensuring better generalization to make the model more robust and scalable for practical deployment.

5.3 Implication for Further Study

The findings highlight key areas for further research and model optimization. While the model demonstrates strong classification performance, its high evaluation runtime and low inference speed indicate a need for computational efficiency improvements. Future studies could explore optimization techniques such as model quantization, pruning, or using more efficient architectures like knowledge distillation to reduce inference time without compromising accuracy. Additionally, given the observed signs of overfitting, further research should focus on improving the model's generalization capabilities. Investigating advanced regularization techniques, data augmentation strategies, or transfer learning approaches could help mitigate overfitting and enhance performance on unseen data.

Moreover, expanding the dataset with more diverse and representative samples could improve model robustness, particularly in handling real-world variations in input data. Exploring alternative loss functions or fine-tuning hyperparameters may also yield performance enhancements. Lastly, integrating explainability techniques such as SHAP or

LIME could provide deeper insights into model decisions, enabling better interpretability for healthcare applications or other critical domains. Addressing these areas will contribute to making the model more scalable, efficient, and reliable for real-world deployment.

References

[1] Zhang, H., Zhou, Y., Zhang, Z., Sun, H., Pan, Z., Mou, M., Zhang, W., Ye, Q., Hou, T., Li, H., Hsieh, C.-Y., & Zhu, F. (2024). Large Language Model-Based Natural Language Encoding Could Be All You Need for Drug Biomedical Association Prediction. Analytical Chemistry. https://doi.org/10.1021/acs.analchem.4c01793

[2] Liang, Y., Zhang, R., Li, Y. G., Huo, M., Ma, Z., Singh, D., Gao, C., Rahmani, H., Bandi, S., Zhang, L., Weinreb, R. N., Malhotra, A., Grotjahn, D. A., Awdishu, L., Ideker, T., Gilson, M. K., & Xie, P. (2024). Multi-Modal Large Language Model Enables All-Purpose Prediction of Drug Mechanisms and Properties. https://doi.org/10.1101/2024.09.29.615524

[3] Alshehri, B. M. J., Kraïem, N., Sakly, H., & Alasbali, N. (2024). Enhancing Medication Safety with Large Language Models: Advanced Detection and Prediction of Drug-Drug Interactions. https://doi.org/10.1109/atsip62566.2024.10638993

[4] Qiu, J., Xiao, Y., Tian, Y., Li, Q., Liu, X., Yang, Y., Tong, H. H. Y., & Liu, H. (2024). PTB-DDI: An Accurate and Simple Framework for Drug–Drug Interaction Prediction Based on Pre-Trained Tokenizer and BiLSTM Model. International Journal of Molecular Sciences. https://doi.org/10.3390/ijms252111385

[5] Aydın, S., Karabacak, M., Vlachos, V., & Margetis, K. (2025). Navigating the potential and pitfalls of large language models in patient-centered medication guidance and self-decision support. Frontiers in Medicine. https://doi.org/10.3389/fmed.2025.1527864

[6] Alshehri, B. M. J., Kraïem, N., Sakly, H., & Alasbali, N. (2024). Enhancing Medication Safety with Large Language Models: Advanced Detection and Prediction of Drug-Drug Interactions. https://doi.org/10.1109/atsip62566.2024.10638993

[7] Xu, T., & Li, B. (2025). KELLM: Knowledge-Enhanced Label-Wise Large Language Model for Safe and Interpretable Drug Recommendation. Electronics. https://doi.org/10.3390/electronics14010154

[8] Xu, C., Bulusu, K. C., Pan, H., & Elemento, O. (2024). DDI-GPT: Explainable Prediction of Drug-Drug Interactions using Large Language Models enhanced with Knowledge Graphs. https://doi.org/10.1101/2024.12.06.627266

[9] Wang, T., Deng, Q., Hu, J., Wang, Y., Peng, J., Chen, J., & Shang, X. (2024). A multi-scale feature fusion model based on biological knowledge graph and transformer-encoder for drug-drug interaction prediction. bioRxiv. https://doi.org/10.1101/2024.01.12.575305

[10] Lin, J., Wu, L., Zhu, J., Liang, X., Xia, Y., Xie, S., Qin, T., & Liu, T.-Y. (2022). R2-DDI: relation-aware feature refinement for drug-drug interaction prediction. Briefings in Bioinformatics. https://doi.org/10.1093/bib/bbac576

[11] C. Xu, K. C. Bulusu, H. Pan, and O. Elemento, “DDI-GPT: Explainable Prediction of Drug-Drug Interactions using Large Language Models enhanced with Knowledge Graphs,” Dec. 2024, doi: 10.1101/2024.12.06.627266.

[12] B. M. J. Alshehri, N. Kraïem, H. Sakly, and N. Alasbali, “Enhancing Medication Safety with Large Language Models: Advanced Detection and Prediction of Drug-Drug Interactions,” pp. 547–552, Jul. 2024, doi: 10.1109/atsip62566.2024.10638993.

[13] Y. Dou, X. Zhao, H. Zou, J. Xiao, X. Peng, and S. Peng, “ShennongGPT: A Tuning Chinese LLM for Medication Guidance,” Nov. 2023, doi: 10.1109/medai59581.2023.00017.

[14] Y. Dou et al., “ShennongMGS: An LLM-based Chinese Medication Guidance System,” ACM transactions on management information systems, Apr. 2024, doi: 10.1145/3658451.

[15] B. Vasantha, B. R. Rakshitha, B. Ankitha, D. S. MEGHANA, and G. A. Nikitha, “Detecting side effects of adverse drug reactions through drug-drug interactions using graph neural networks and selfsupervised learning,” Journal of Nonlinear Analysis and Optimization: Theory & Applications, vol. 15, no. 02, pp. 179–185, Jan. 2024, doi: 10.36893/jnao.2024.v15i12.048.

[16] F. Cheng, V. Zouhar, R. Chan, D. Fürst, H. Strobelt, and M. El-Assady, “Interactive Analysis of LLMs using Meaningful Counterfactuals,” Apr. 2024, doi: 10.48550/arxiv.2405.00708.

[17] N.-N. Wang, B. Zhu, X.-L. Li, S. Liu, J.-Y. Shi, and D. Cao, “Comprehensive Review of Drug-Drug Interaction Prediction Based on Machine Learning: Current Status, Challenges, and Opportunities,” Journal of Chemical Information and Modeling, Dec. 2023, doi: 10.1021/acs.jcim.3c01304.

[18] Drug-Drug Interactions and Side Effects Prediction Using Shallow Ensemble Deep Neural Networks,” in Lecture notes in electrical engineering, 2022, pp. 377–387. doi: 10.1007/978-981-19-2281-7_36.

[19] J. Li, Y. Wang, Z. Li, H. Lin, and B. Wu, “LM-DTI: a tool of predicting drug-target interactions using the node2vec and network path score methods,” Frontiers in Genetics, vol. 14, May 2023, doi: 10.3389/fgene.2023.1181592.

Department of Computer Engineering
Marwadi University

Academic Year: 2024-25

Semester: 8

Major Project-II (01CE0807)

Weekly Progress Report Diary (Project)

Team ID: 8CE_P010

Project Title: *MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant*

Sr. No.	Student Full Name	Student En. No.	Class
1	Masruk Habib	92100103165	TC-1
2	Puvanenthira Raja	92100103168	TC-1

Internal Guide Name: *Ravikumar R N*

Weekly Project Progress Report Diary – January

Week	Project Activity by Students	Updates / Comments / Suggestions / Remarks by Faculty	Date & Time	Guide Signature
1				
2				
3				
4				

Weekly Project Report Diary – FEBRUARY

Week	Project Activity by Students	Updates / Comments / Suggestions / Remarks by Faculty	Date & Time	Guide Signature
1				
2				
3				
4				

Weekly Project Report Diary – MARCH

Week	Project Activity by Students	Updates / Comments / Suggestions / Remarks by Faculty	Date & Time	Guide Signature
1				
2				
3				
4				

Weekly Project Report Diary – APRIL

Week	Project Activity by Students	Updates / Comments / Suggestions / Remarks by Faculty	Date & Time	Guide Signature
1				
2				
3				
4				

Consent for Filing Patent/Research Publication Application

We, **Ravikumar R N**, **Masruk Habib, Puvanenthirarajah,** hereby give our full consent and authorization for the filing of a patent/research publication application for the project titled **" MediGuard AI: An Interactive Drug and Side Effect Predictor Using LLMs with a RAG-Based Chat Assistant**".

We hereby authorize Marwadi University and/or its legal representatives to file the patent/research publication application and act on our behalf regarding any matters related to this filing.

Date: 04.04.2025
Name: Ravikumar R N
Signature:

Date: 04.04.2025
Name: Masruk Habib
Signature:

Date: 04.04.2025
Name: Puvanenthirarajah
Signature: