Construction of a Dataset for Automated Prescription Recommendations: A Focus on Antibiotic Drug Interactions using Retrieval-Augmented Generation

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Abstract. This project seeks to construct a comprehensive dataset to support automated prescription recommendations, with a particular emphasis on antibiotic drug interactions.
By employing a Retrieval-Augmented Generation (RAG) approach and Large Language Models (LLMs), the dataset aims to enhance the precision and contextual awareness of AI-driven decision-making in medical prescriptions. This paper presents the objectives of the project, a review of related work, and the methodologies that will be applied to achieve the goal.

Keywords: Dataset Construction, Automated Prescription, Retrieval-Augmented Generation, Large Language Models, Antibiotic Drug Interactions, AI in Medicine

1 Aims

This study aims to develop a structured and comprehensive database regarding antibiotics and their interactions with medications, including interactions with other antibiotics and frequently prescribed medications in clinical settings.

The primary objective is to leverage this curated dataset to implement Retrieval-Augmented Generation (RAG) and Large Language Models (LLMs) within an AI-powered medical prescription support system. By utilizing advanced natural language processing techniques, the system will retrieve and generate contextualized recommendations for antibiotic prescriptions while prioritizing patient safety and mitigating the risks associated with adverse drug interactions.

This study likewise focuses on assessing the efficacy of Retrieval-Augmented Generation (RAG) -enhanced Large Language Models (LLMs) to improve the accuracy, consistency, and interpretability of prescription recommendations compared to conventional decision-support tools. By developing a comprehensive knowledge base and incorporating artificial intelligence-driven methodologies, this research aspires to advance intelligent healthcare systems, thereby enabling more informed decision-making processes for healthcare professionals and promoting the safer and more effective utilization of antibiotics in clinical practice.

2 State of the Art

2.1 Antibiotics-Drug Interactions

A drug–drug interaction (DDI) refers to a phenomenon in which the presence of one medication alters the effects of another, potentially reducing its efficacy, increasing toxicity, or, in severe instances, leading to fatal outcomes [25].

Antibiotic-drug interactions (ADIs) specifically involve these alterations when one of the drugs in question is classified as an antibiotic. ADIs are a critical area of research due to the widespread use of antibiotics and the pharmacokinetic and pharmacodynamic mechanisms that make them significant contributors to Adverse Drug Reactions (ADRs) [11]. An antibiotic failure is a serious concern, as interactions not only affect the effectiveness of antibiotics but also contribute to antibiotic resistance [3].

These issues occur more frequently in vulnerable populations such as children, the elderly, and individuals with chronic diseases. This heightened risk is attributed to polypharmacy, multiple comorbidities, regular off-label medication usage, and specific dosage regimens [2].

Given the growing multidrug resistance demonstrated by bacteria to nearly all classes of antibiotics, it is extremely beneficial to create a comprehensive database that thoroughly documents all potential adverse drug interactions (ADIs) [10].

Furthermore, advances in computational methods, especially artificial intelligence (AI), provide significant potential to improve the detection and management of ADIs in clinical practice.

2.2 AI in Medical Prescription Recommendation Systems

The creation of medical prescription recommendation systems designed to forecast and avert ADIs is a vital research focus, particularly as antibiotic resistance and adverse drug events become increasingly concerning.

These systems aim to enhance antibiotic usage while reducing harmful interactions.

Numerous studies have investigated the application of machine learning for predicting antibiotic combinations and their interactions. An antibiotic combination recommendation model (ACRM) was developed using a machine learning algorithm, demonstrating acceptable clinical relevance and accuracy in predictions, which suggests its potential to mitigate drug interactions [10].

Another study employed a label propagation framework to predict DDIs by integrating clinical side effects and chemical structures, showcasing the efficacy of computational models in forecasting harmful effects DDIs [22].

The PARS system combines semantic technologies with Multiple Criteria Decision Aiding (MCDA) to support antibiotic prescriptions. Its ability to dynamically update a patient's profile and integrate new information makes it more adaptable and reliable compared to static guidelines [13]. Similarly, AntibioHelp® functions as a clinical decision support tool that assists general practitioners in interpreting guidelines for patients without clear recommendations, ultimately boosting prescription confidence [17].

Frameworks that utilize molecular structure descriptors have been developed to effectively predict antibiotic interactions. These models can accurately anticipate interactions based on chemical structures, which helps in identifying drug pairs that work synergistically. [7]

Additionally, semi-mechanistic pharmacokinetic-pharmacodynamic (PKPD) models have been used to suggest optimal dosing regimens for antibiotic combinations, effectively addressing variability and uncertainty in parameters.[4]

2.3 Role of Large Language Models in Prescription Recommendations

Large Language Models (LLMs) exhibit considerable potential for enhancing Medical Prescription Recommendation Systems, as indicated by Sridharan (2024). This advancement has the capacity to fundamentally alter the techniques employed in prescribing and managing medications.

LLMs are sophisticated artificial intelligence models trained on vast amounts of text data, enabling them to understand and generate human-like language. They possess strong logic and reasoning skills and general world knowledge. Their capabilities extend to various Natural Language Processing (NLP) tasks, including understanding, summarization, question answering, creative writing, and even code generation [12].

In healthcare, LLMs present promising applications such as medication review and reconciliation where LLMs can assist in identifying dosing regimen errors, drug-drug interactions, and suggesting dosage adjustments based on therapeutic drug monitoring and genomics. Studies have assessed the abilities of models like ChatGPT, Claude-Instant, and Gemini in these processes, noting their potential to revolutionize medication management.[14]

Clinical decision-making represents an additional domain in which LLMs can assist in the synthesis and analysis of patient data, enhance communication between patients and healthcare providers, and support the clinical decision-making process.[20]

In pharmacology and drug discovery, LLMs can transform knowledge query methods, enabling multi-round consultations on pharmacological questions. They can assist with drug property queries, lead compound structure optimization, and summarizing research trends and limitations.[9]

Personalized prescriptions using open-source LLMs, especially when combined with Retrieval-Augmented Generation (RAG), are being evaluated for their ability to generate tailored, patient-specific medication prescriptions [1].

However,LLMs face several limitations, including hallucinations that generate incorrect or misleading information [15], particularly in specific domains without real-time data. Outdated knowledge from old training datasets can also hinder accuracy [18]. To mitigate these issues, RAG has been proposed to enhance the medical question-answering capabilities of LLMs with external knowledge bases; however, it may still fail in complex cases where multiple rounds of information-seeking are required [19].

Furthermore, interacting with LLM can be computationally costly, which complicates the accuracy of complex tasks [24]. Ethical concerns arise from potential misuse, lack of transparency, and issues regarding patient privacy and informed consent [12].

2.4 Retrieval-Augmented Generation (RAG)

Retrieval-Augmented Generation (RAG) represents a methodological advancement aimed at augmenting the functionality of LLMs through the integration of pertinent information derived from an external database during the text generation process [8].

This approach alleviates hallucinations by grounding responses in factual sources [6]. In addition, RAG expands the model's knowledge base by integrating current information, such as new research and clinical guidelines, with frameworks like Almanac [21] and MedRAG [19] to ensure more informed and contextually relevant output.

Studies show that RAG-enhanced LLMs consistently outperform standard models in terms of accuracy and evaluation metrics, such as iDISK2.0 [5], in the context of dietary supplements.

Furthermore, it improves transparency by facilitating source attribution, which allows users to verify the origins of retrieved information- an essential feature in fields such as medicine and scientific research, where credibility is crucial [23].

For elderly patients, it helps with medication management by cross-referencing curated datasets like DrugBank [16].

Additionally, systems like Chat2Data [24] utilize RAG to augment domain knowledge, enabling more efficient and low-code data analysis.

3 Problem Analysis and Methodology

A critical challenge in healthcare is predicting and detecting potential interactions between antibiotics and other drugs, particularly in patients with comorbidities who are undergoing complex medication regimens. These patients face a heightened risk of experiencing harmful interactions, which can result in adverse effects, treatment failures, and antibiotic resistance. Although general-purpose LLMs show some capability in identifying drug interactions, they frequently overlook specific interactions or yield incorrect data, posing risks in clinical environments. This highlights the necessity for specialized models designed to accurately detect ADIs and offer trustworthy guidance. The system will depend on the following methodologies:

- **Data collection and Structuring:** Data will be collected from various sources, including DrugBank. This collection will encompass information about medications, interactions, adverse effects, and clinical guidelines.
- **Indexing:** External data is transformed into vector embeddings—numerical representations—and stored in a vector database for efficient retrieval.
- **Information Retrieval:** When a user submits a query, the system retrieves relevant documents using semantic search, ensuring content aligns with the query's context.
- **Generation with LLMs:** After retrieving relevant data, an LLM generates prescription recommendations aligned with clinical practices.

4 Work Plan

The project will be divided into the following stages:

- **Stage 1: Data Collection and Preparation**: Compile and preprocess the necessary datasets.
- **Stage 2: System Development**: Develop the retrieval and generation pipeline using RAG and LLMs.
- **Stage 3: Testing and Evaluation**: Conduct testing and evaluate the system's ability to generate accurate and clinically relevant prescriptions.
- **Stage 4: Final Report and Presentation**: Write the final article and prepare the presentation for the project.

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