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Research Article

A User-Interface to Trace, Map and Resolve Drug-Drug Interactions

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Abstract

The increasing use of multiple medications in chronic disease management has raised concerns about drug–drug interactions (DDIs) and their impact on patient safety. This challenge is particularly significant in health conditions such as diabetes, which often associates with comorbidities like increased blood pressure, hyperlipidemia, and heart ailments. Such health conditions and their comorbidities require complex multi-drug regimens or polypharmacy. Drug–Drug Interaction (DDIs) occurs when one drug interferes with the pharmacodynamic or pharmacokinetic functions of the other drug, potentially leading to severe toxicity or treatment failure. Such interactions are a major contributor to hospital admissions, and the associated risks escalate as the number of medications increases. This research work, presents a clinical decision-support system which analyzes DDI of multi-drug combinations. It also calculates the overall DDI risk, identifying the risk-contributing drug and suggesting its safer therapeutic alternative. By converting DDI interaction analysis into clear and actionable guidance, this system helps in selecting safer drug combinations and supports better clinical decision-making.

Keywords: Drug–Drug Interaction (DDIs); Graph Neural Network (GNN)

Introduction

The rising prevalence of chronic conditions requiring polypharmacy raises a critical safety question regarding whether complex drug combinations are truly safe for patients. A drug–drug interaction (DDI) occurs when two or more drugs interfere with each other's biological actions, potentially leading to severe toxicity or treatment failure. Such interactions are a major contributor to hospital admissions, and the associated risks escalate as the number of medications increases.

Unfortunately, existing DDI monitoring systems are often limited by their reliance on pairwise analysis, which fails to capture the cumulative effects of multi-drug combinations. Additionally, such systems provide a basic interaction warning, lacking the much-needed active decision support of identifying the risk-contributing drug(s) and its recommended, safer therapeutic, alternate. Hence, there is a need for a polypharmacy-risk monitoring system that focuses on common health conditions with frequent comorbidities, for example diabetes necessitating multifaceted drug regimens.

Methodology

To overcome the above mentioned challenge of polypharmacy risk, we developed a Graph Neural Network (GNN) for predicting DDI risk. By using the DDI risk predictions we have developed a user interface for enhanced clinical utility. Following is the process flow for the methodology:

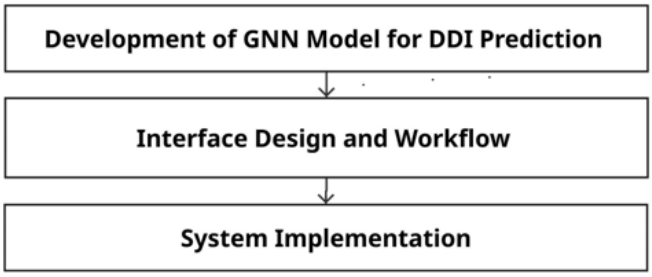

Figure 1: Overall system workflow.

The workflow illustrates the overall methodology, starting from GNN-based DDI prediction, followed by interface design and decision-support workflow, and concluding with system implementation for real-time risk assessment and recommendation.

Development of GNN model for DDI prediction

A Graph Neural Network (GNN) is used to integrate diverse biological datasets and learn complex interaction patterns between drugs. To address the lack of reliable negative samples, a Positive–Unlabeled (PU) learning approach is employed to identify high-confidence non-interactions and improve prediction reliability. The model is trained on curated interaction data and evaluated using standard performance metrics to ensure robustness. Ultimately, the model outputs a quantitative interaction score that has been validated against clinical literature to ensure accurate and biologically meaningful results.

The interaction scores predicted by the GNN model are then used by the interface for further risk analysis and decision support, enabling translation of model outputs into clinically interpretable insights.

Interface design and workflow

The interface and workflow are designed to provide actionable decision support by assessing the cumulative risk of a full drug regimen. The system processes user input and translates model predictions into clinically interpretable outputs.

- **Design Objectives:** The interface is designed to provide a simple interaction flow, clear risk interpretation, and actionable decision support.
- **User Input Module:** The user inputs 2 or more drugs for multiple co-morbid conditions.
- **Interaction Analysis:** System computes interaction scores for all drug pairs (e.g., A–B, B–C, A–C).
- **Overall Risk Assessment:** Pairwise scores are aggregated to calculate the overall regimen risk (low, moderate, or high).
- **Problem Drug Identification**: A drug is flagged as problematic if it appears in a high-risk pairwise interaction.
- **Alternative Drug Suggestion:** Alternatives are selected from the same drug class and re-evaluated.
- **Recommended Combination Output:** The combination resulting in the lowest overall risk is recommended as the safer prescription option.

System implementation

To enable practical use of the proposed workflow, the system utilizes interaction scores generated by the GNN model for drug pairs. These scores are accessed by the interface and used for further analysis and decision support. Based on the evaluated results, the interface presents interaction risk along with suggested safer alternatives. The final outputs are displayed through the web interface, enabling efficient processing and real-time response.

Result and Finding

Use case demonstration

- **Input**: The user selects four drugs: Metformin, Gliclazide, Rosuvastatin, and Empagliflozin that are commonly used for diabetes and related conditions such as cholesterol, hypertension, and cardiovascular disease.
- **Analysis**: The system calculates interaction scores for all drug pairs. A high-risk interaction is observed between Metformin and Gliclazide (score: 0.970), while other pairs, such as Metformin–Rosuvastatin (0.060) and Metformin–Empagliflozin (0.207), show low risk, as shown in Figure 1. Based on these values, the overall risk of the combination is classified as MODERATE.

- **Problem Drug Identification**: Since Gliclazide and Metformin are involved in the high-risk interaction, they are identified as the main problem drugs contributing to the increased risk, as shown in Figure 2.

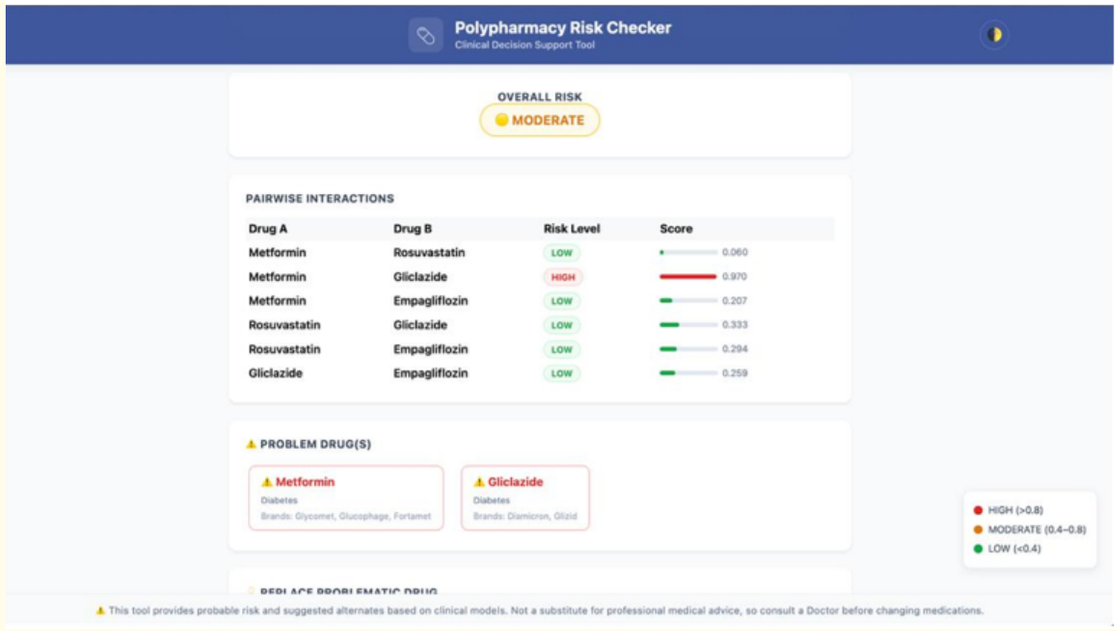

Figure 2: Pairwise interaction analysis and Identification of problem drugs.

Pairwise interaction scores for the selected drugs highlight a high-risk interaction (0.970) between Metformin and Gliclazide, leading to overall MODERATE risk and identification of problem drugs.

- **Recommendation**: The system suggests replacing Gliclazide with Saxagliptin, a drug from the same class. The updated combination: Metformin, Saxagliptin, Rosuvastatin, and Empagliflozin is then re-evaluated and classified as LOW risk, indicating a safer option as shown in Figure 3.

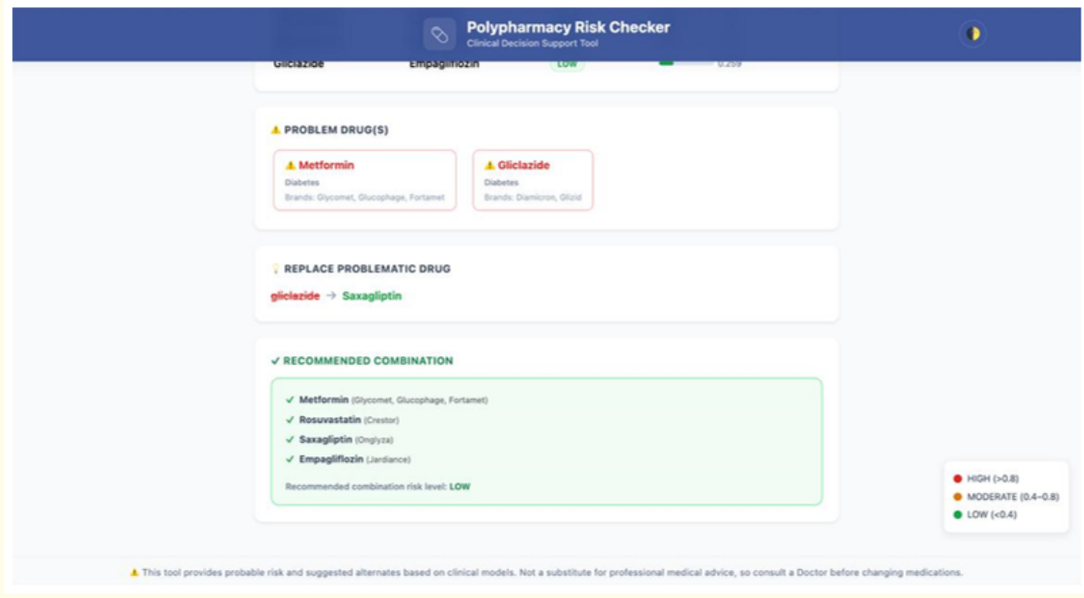

Figure 3: Alternative recommendation.

Gliclazide is replaced with Saxagliptin, and the updated combination is re-evaluated as LOW risk, providing a safer alternative.

If the suggested replacement also results in a high-risk interaction with other drugs in the combination, the system evaluates additional alternatives and recommends the option with the lowest overall risk.

The model achieved high predictive performance (ROC-AUC: 0.980, F1 Score: 0.965), and the predicted high-risk interactions are consistent with clinical evidence, supporting the reliability of the results.

Discussion

This integrated system provides a practical approach for optimizing long-term disease management in complex clinical settings. By moving from passive interaction detection to active decision support, the platform enables clinicians to identify problematic drugs and evaluate safer alternatives. This reduces reliance on manual interpretation of interaction warnings and supports faster, more reliable clinical decision-making. Furthermore, the proposed framework is adaptable and can be extended to other disease conditions and varying drug combinations, highlighting its potential for broader clinical applicability [1-3].

Conclusion

Our framework successfully integrates a GNN prediction model with a clinical decision-support interface. By accurately assessing polypharmacy risk, identifying the drug(s) most responsible for adverse interactions, and recommending safer therapeutic alternatives, the system transforms interaction detection into active clinical support. This approach holds significant potential to enhance patient safety and optimize treatment plans in complex clinical environments.

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