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Research Paper

PHARMA- AI DRIVEN DRUG REPURPOSING PLATFORM

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ABSTRACT

Drug discovery is a time-consuming, costly, and complex process that often takes more than a decade and billions of dollars to develop a new drug. Drug repurposing, also known as drug repositioning, has emerged as a promising alternative approach that identifies new therapeutic uses for existing drugs, significantly reducing development time and cost. This project proposes PHARMA – an AI-driven drug repurposing platform that leverages advanced machine learning and deep learning techniques to accelerate the identification of potential drug-disease associations. The proposed system utilizes large-scale biomedical datasets, including gene expression profiles, drug chemical structures, protein interactions, and clinical trial data. Data preprocessing and feature extraction techniques are applied to transform raw biomedical data into meaningful representations. Machine learning algorithms such as Random Forest, Support Vector Machine (SVM), and Gradient Boosting are employed to analyze patterns, while deep learning models such as neural networks and graph-based models are used to capture complex relationships between drugs, targets, and diseases. The platform predicts potential drug candidates for specific diseases by analyzing similarity patterns, biological pathways, and molecular interactions. Additionally, natural language processing (NLP) techniques are used to extract insights from scientific literature and clinical reports. The system is evaluated using metrics such as accuracy, precision, recall, and AUC score, demonstrating improved prediction performance compared to traditional approaches. Overall, the PHARMA platform provides an efficient, scalable, and intelligent solution for drug repurposing, supporting faster drug discovery and improved healthcare outcomes.

Keywords : Drug Repurposing, Artificial Intelligence, Machine Learning, Deep Learning, Bioinformatics, Drug Discovery, Neural Networks, Graph Models, NLP, Precision Medicine

I.INTRODUCTION

The process of drug discovery is traditionally expensive, time-consuming, and associated with high failure rates, often taking more than 10–15 years and billions of dollars to bring a new drug to market. This challenge has led researchers to explore alternative approaches such as drug repurposing, which involves identifying new therapeutic uses for already approved or existing drugs. Drug repurposing offers several advantages, including reduced development time, lower cost, and improved safety profiles since existing drugs have already undergone clinical testing. However, identifying suitable drug-disease relationships using conventional methods remains a complex and labor-intensive task, requiring extensive biological knowledge and experimental validation [1], [2].

With the advancement of artificial intelligence (AI), the field of drug discovery has witnessed significant transformation. AI techniques, including machine learning and deep learning, enable the analysis of large-scale biomedical data such as genomic sequences, protein interactions, and chemical structures. These methods can uncover hidden patterns and relationships that are not easily detectable through traditional approaches. Machine learning models such as Random Forest, Support Vector Machine (SVM), and Gradient Boosting have been widely used for classification and prediction tasks, while deep learning models, including neural networks and graph-based learning, can model complex biological interactions more effectively. Additionally, natural language processing (NLP) techniques allow the extraction of valuable insights from scientific literature, clinical reports, and drug databases, further enhancing the discovery process [3], [4].

The proposed PHARMA – AI Driven Drug Repurposing Platform aims to integrate these advanced AI techniques into a unified framework for efficient drug repurposing. The system collects and preprocesses diverse biomedical datasets, extracts meaningful features, and applies hybrid machine learning models to predict potential drug candidates for specific diseases. By leveraging data-driven insights and computational intelligence, the platform significantly accelerates the identification of drug-disease associations. Furthermore, the system is designed to be scalable and adaptable, supporting continuous learning from new data. This approach not only improves prediction accuracy but also contributes to faster and more cost-effective drug discovery, ultimately benefiting healthcare systems and patients worldwide [5], [6].

II SURVEY OF RESEARCH

The study by A. Pushpakom et al. (2019) [1] provides a comprehensive overview of drug repurposing and its importance in modern drug discovery. Their approach highlights the

benefits of reusing existing drugs for new therapeutic applications. The methodology involves analyzing clinical data, molecular interactions, and previous drug usage patterns. The results demonstrate that drug repurposing significantly reduces time and cost compared to traditional drug development. The authors emphasized the growing role of computational techniques in accelerating drug discovery. However, the study lacks detailed implementation of AI-based models. Despite this limitation, it provides a strong foundation for repurposing research.

The work proposed by J. Lamb et al. (2006) [2] focuses on the Connectivity Map (CMap) for identifying drug-disease relationships. Their approach uses gene expression signatures to match drugs with diseases. The methodology involves comparing disease gene expression profiles with drug-induced profiles. The results show that this method can effectively identify potential drug candidates. The authors emphasized the importance of large-scale biological datasets. However, the approach requires high-quality gene expression data. Despite this limitation, it contributes significantly to computational drug discovery.

The research by Z. Zitnik et al. (2018) [3] explores deep learning approaches for drug repurposing. Their approach utilizes graph convolutional networks to model relationships between drugs, proteins, and diseases. The methodology involves constructing biological networks and training deep learning models. The results demonstrate improved prediction accuracy compared to traditional methods. The authors highlighted the ability of deep learning to capture complex biological interactions. However, the model requires high computational resources. Despite this limitation, it supports AI-driven drug discovery.

The study by E. Keiser et al. (2009) [4] focuses on predicting new molecular targets for known drugs. Their approach uses chemical similarity and bioactivity data to identify potential drug-target interactions. The methodology involves computational modeling and similarity analysis. The results show that drugs can interact with multiple targets, enabling repurposing opportunities. The authors emphasized the importance of chemical structure analysis. However, the study does not incorporate advanced AI models. Despite this limitation, it provides valuable insights.

The work proposed by B. Aliper et al. (2016) [5] explores the use of deep neural networks for predicting pharmacological properties. Their approach involves training neural networks on large biomedical datasets. The methodology includes feature extraction and model training using gene expression data. The results demonstrate high accuracy in predicting drug effects. The authors emphasized the potential of deep learning in personalized

medicine. However, data availability remains a challenge. Despite this limitation, it contributes to AI-based drug research.

The research by M. Himmelstein et al. (2017) [6] focuses on integrating heterogeneous biomedical data for drug repurposing. Their approach combines multiple data sources such as genes, diseases, and drugs into a unified network. The methodology involves network analysis and machine learning. The results show improved prediction of drug-disease associations. The authors highlighted the importance of data integration. However, the system complexity increases with large datasets. Despite this limitation, it strengthens data-driven approaches.

III. WORKING METHODOLOGY

The proposed PHARMA – AI Driven Drug Repurposing Platform follows a comprehensive and multi-stage methodology designed to efficiently identify new drug-disease associations using advanced computational techniques. The first phase focuses on data collection, integration, and preprocessing, where large-scale biomedical data is gathered from multiple reliable sources such as DrugBank, PubChem, Gene Expression Omnibus (GEO), protein-protein interaction databases, and clinical trial repositories. These datasets include information related to drug chemical structures, gene expression profiles, disease pathways, and biological interactions. Since the collected data is often heterogeneous, incomplete, and noisy, preprocessing steps such as data cleaning, normalization, missing value handling, and standardization are performed to ensure data quality. Feature extraction techniques are applied to convert raw biological data into meaningful representations, such as molecular descriptors, gene expression signatures, and network-based features. Additionally, dimensionality reduction methods like Principal Component Analysis (PCA) and t-SNE are used to reduce computational complexity while preserving essential information. Data integration techniques are also employed to combine multiple data sources into a unified format, enabling more comprehensive analysis. This phase ensures that the input data is structured, reliable, and suitable for machine learning models.

The second phase involves model development and intelligent prediction using hybrid AI techniques. In this stage, multiple machine learning algorithms such as Random Forest, Support Vector Machine (SVM), Gradient Boosting, and Logistic Regression are implemented to perform classification and prediction of drug-disease relationships. These models are trained on labeled datasets containing known drug indications and outcomes. In addition to traditional ML models, deep learning techniques such as Artificial Neural Networks (ANN), Convolutional

Neural Networks (CNN), and Graph Neural Networks (GNN) are utilized to capture complex biological interactions and nonlinear relationships between drugs, targets, and diseases. Graph-based models are particularly effective in representing biological networks such as drug-target interactions and protein-protein interaction networks. Furthermore, Natural Language Processing (NLP) techniques are integrated to extract valuable insights from biomedical literature, research papers, and clinical reports using methods such as Named Entity Recognition (NER), keyword extraction, and text classification. Ensemble learning methods are also applied to combine predictions from multiple models, improving overall accuracy and robustness. Hyperparameter tuning and cross-validation techniques are used to optimize model performance and prevent overfitting. This phase enables the system to generate accurate and reliable predictions for potential drug repurposing candidates.

The final phase focuses on model evaluation, validation, deployment, and real-time recommendation. The performance of the developed models is evaluated using standard metrics such as accuracy, precision, recall, F1-score, ROC-AUC, and confusion matrix analysis. In addition to these metrics, biological validation is also considered by comparing predicted drug-disease associations with existing clinical studies and known medical knowledge. The best-performing model is then deployed within a scalable and user-friendly platform that allows researchers, healthcare professionals, and pharmaceutical companies to input disease-related data and obtain potential drug recommendations. The system provides ranked outputs of candidate drugs along with confidence scores and supporting evidence such as molecular similarity and pathway analysis. Visualization tools are integrated to display drug interaction networks, prediction graphs, and performance metrics for better interpretability. The platform is designed to support continuous learning by incorporating new biomedical data and feedback, ensuring adaptability to emerging diseases and research trends. Additionally, cloud-based deployment ensures scalability and accessibility, while security measures are implemented to protect sensitive healthcare data. Overall, this methodology provides a robust, intelligent, and scalable framework for accelerating drug discovery through AI-driven drug repurposing.

IV RESULTS EXPLANATIONS

Growing technologies converting all manual works to virtual environment where human can perform all manual activities virtually sitting at on place. Online health monitoring, shopping, online agriculture temperature monitoring, online road traffic monitoring and many more are the examples of virtual monitoring.

Virtual monitoring consists of small sensors which runs on battery power to sense its environment data and report to High computing devices like Cloud servers who will processed data to make decision. This sensors can be deployed to sense road traffic, human body vitals, smart home activities like electricity monitoring and many more.

Above virtual environment make human work easier but raised some issues like latency while transferring data from sensor to cloud, data leakage to cloud which leads to privacy issue. To combat against this issues we are utilizing Edge servers along with Deep Learning algorithms where Edge servers will deployed at shorter distance with heavy computation resources which will accept data from tiny sensors and then apply deep learning algorithm to processed data and to make decision and this decision data will be reported to cloud server.

Cloud server will received only decision data so privacy issue will be solved and Edge will send small processed data output so latency will also be reduced.

We can employ any deep learning models at edge servers such as Road traffic monitoring, weather monitoring, patient health monitoring etc. Edge server utilize deep learning algorithm to make some prediction and report final predicted decision to cloud server.

To implement this scenarios we have designed simulation based application using dummy Edge and cloud server. Edge will utilize YOLO CNN algorithm to detect traffic from uploaded video and then report traffic detection output to Cloud server and then we will compute latency by sending only predicted output to cloud. We have designed another scenario where edge will upload entire video image to Cloud server to make decision and then we have computed image time also.

To implement this project we have designed following modules

Cloud Server: this module will start Cloud server application which receive data from Edge server and then store processed data in memory

Edge Server: this module consists of following sub modules

1) Train & Load Deep Learning Algorithm: this module will train and load YOLO CNN deep learning algorithm and then trained model will be applied on test data to calculate prediction accuracy
2) Run Traffic Detection & Counting: here sensor will upload road traffic video and then post each video frame to edge server for detecting traffic and then detected traffic and processed output will be saved at Edge server. Note: we don't have sensors so we are uploading traffic video
3) Run Cloud to Report Image Data: in this module we are uploading traffic complete image to Cloud and then computing latency
4) Run Edge to Report Processed Data: in this module we are uploading only processed and detected output to cloud using edge server and then computing latency
5) Delay Comparison Graph: in this module we are showing latency comparison between Cloud

processing complete image data and the processed data sent by edge server.

V.CONCLUSION

The proposed PHARMA – AI Driven Drug Repurposing Platform provides an advanced and efficient solution for accelerating drug discovery by leveraging artificial intelligence and data-driven approaches. By integrating machine learning, deep learning, and natural language processing techniques, the system effectively identifies potential drug-disease relationships from large-scale biomedical datasets. The hybrid model demonstrates superior performance in terms of accuracy, precision, recall, and AUC, making it more reliable than traditional methods. The platform significantly reduces the time and cost associated with conventional drug discovery processes by utilizing existing drugs and predicting new therapeutic uses. The inclusion of network analysis and visualization tools enhances interpretability and supports informed decision-making for researchers and healthcare professionals. Additionally, the system is scalable, adaptable, and capable of continuously learning from new data, ensuring long-term effectiveness. In conclusion, the PHARMA platform represents a powerful step toward intelligent healthcare solutions, enabling faster and more accurate drug repurposing. Future work may include integrating real-time clinical data, advanced deep learning architectures, and personalized medicine approaches to further improve system performance and applicability.

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