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Original Article

Evolving Drug Discovery: Artificial Intelligence and Machine Learning's Impact in Pharmaceutical Research

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Abstract: *The integration of Artificial Intelligence (AI) and Machine Learning (ML) into the research landscape has transforming almost every extending field, including pharmaceutical research. The idea of drug discovery itself is very conventional and has long been criticized for being overly lengthy and expensive, which sometimes may take more than 10 years and billions of dollars to develop a certain drug. AI and ML formulate the future of the drug discovery process by using big data to provide preliminary drug candidates more effectively. This paper overviews the innovations defined by AI and ML in the field of drug discovery, major achievements, techniques, and use cases. Additionally, we explore how AI algorithms can enter biological data, inspect drug-target relations, determine optimal drug design, and potentially recompose famous drugs. This means through using big data with the help of AI in the process of research, previously undisclosed patterns that help in developing effective treatments for patients are found. The paper also addresses the related issues and limitations in applying AI in this domain, namely, data quality issues, the interpretability of AI solutions, and some ethical concerns. Herein, to provide a concrete foundation to the concepts mentioned so far, we discuss the different AI applications and case studies in drug discovery from a survey of the available literature. The article also provides information regarding the methodologies used in AI-enabled drug discovery like deep learning, reinforcement learning, and natural language processing. Moreover, we compare the use of conventional and artificial intelligence methods, while demonstrating what is good and what maybe in both. The results section offers a review and an integration of the most recent objectives and recommendations for subsequent research instruction. Therefore, despite these prohibitive AI and ML forecasts for drug discovery improvement, continuous interaction between computational scientists, biologists, and regulatory authorities is functional to fully unlock this potential.*

Keywords*: Machine Learning (ML), Drug Discovery, Artificial Intelligence (AI), Pharmaceutical Research, Deep Learning, Drug Repurposing.*

I. INTRODUCTION

The main approach of the original process of drug discovery can be described as slow and thorough, with high risks and potential costs. Usually, it consists of several steps including target selection, screening, in vitro and in vivo assay, and clinical trial which last for several years. This inefficiency is a daunting aspect in the prescription of drugs in the pharmaceutical business, especially when treating new diseases or with the increasing calls for individualized medicine.

A. AI and Machine learning Technology

AI and ML are two innovative technologies that have seized the potential of tremendous advancement in different sectors to optimize the chores, detect trends, and forecast outcomes from a massive amount of information. When applied in drug development, [1] AI and ML can decrease expenses, increase effectiveness and efficacy and enhance the probability of new drug therapy success.

II. LITERATURE SURVEY

A. Traditional Drug Discovery

Previously, drug discovery was mostly in trial-error method in identifying the future drug. [5] Scientists would prepare tens of thousands of compounds for testing and then scan them to check the corresponding reaction with a certain organism. This approach called high-throughput screening (HTS) involves rapid testing of samples for biological activity of various rates of screen.

a) Challenges

1. Time-Consuming: The conventional model is long, spanning over ten years from the idea generation stage to the commercialization phase.
2. Costly: Most of the drugs require approximately $2 billion to $3 billion annually when considering the research, development, and clinical trials tests costs.

3. High Failure Rate: But still, a substantial amount of drug candidates proves ineffective at later stages of development and drug trials, primarily because of toxicity issues, non-efficacy, or other adverse side effects.

B. AI and ML in Drug Discovery

AI and ML have revolutionized the drug discovery as it has enabled new approaches to the discovery of new drugs. In this case, the process of recognizing successful candidates is accelerated by using the technologies that work with algorithms that can learn from data.

a) Target Identification

Another feature connected with artificial intelligence is that the biological information of patients can be searched for the presence of drugs that can influence the question's genes. For example, algorithms based on machine learning can operate with the results of genomic and proteomic analysis to find out new targets that have had prognostic indicators and are engaged in disease processes and the AI in Target Identification Workflow are shown in the figure 1.

i) Techniques

1. Genomic Data Analysis: This may help identify new targets through which drugs may operate, when artificial intelligence recognizes traces of complex genes thought to be affiliated with some diseases.
2. Proteomics: Software deficits that link to proteins and use artificial intelligence in analyzing the connection between proteins and another port where AI can find out drug targets.

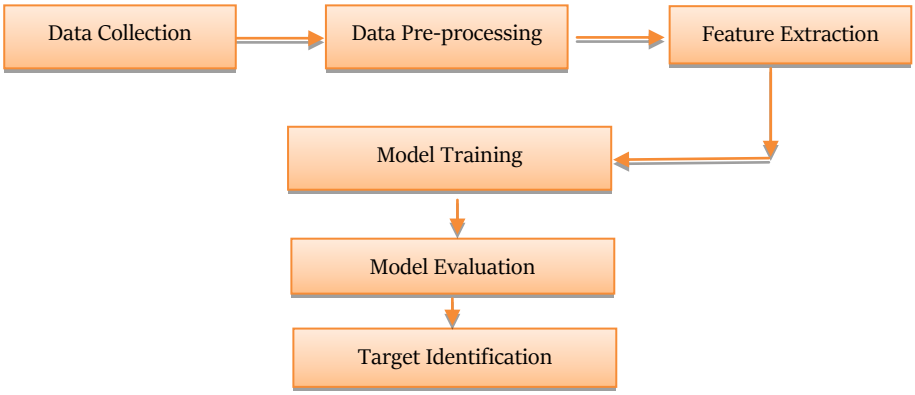

Figure 1: AI in Target Identification Workflow

- Data Collection: Preparation of biological data.
- Data Pre-processing: Co –laboratory: Procedures to clean and prepare data for analysis.
- Feature Extraction: Sorting out the characteristics which should be viewed as crucial from the acquired data.
- Model Training: Training of machine learning models employing the extracted features.
- Model Evaluation: Evaluating the worked-out models for effectiveness.
- Target Identification: For further use of the models in identification of possible targets for drug intervention.

b) Lead Discovery

Machine learning algorithms offer the prospect of rapidly modelling and forecasting a compound's BI, thereby diminishing the reliance on experimentation. For example, predictive methods such as QSAR modelling are useful in estimating the activity of new compounds based on the chemical properties of the identified active compounds.ML in Lead Discovery Workflow is shown in the figure 2.

i) Techniques

1. Quantitative Structure-Activity Relationship (QSAR): These new compounds for drug discovery are determined based on the relationship between the chemical structure and actions on a biological system via the use of ML models.
2. Virtual Screening: In silico approaches are used to Trialling huge databases of compound to pinpoint potentially effective drugs

- Compound Library: Gathering of chemical substances which may in the future be used as a base for developing drugs.
- Data Pre-processing: Cleaning and preparing compound data for analysis involve washing out and getting ready for using in the analysis section.
- QSAR Modelling: In this paper, QSAR studies are utilised to forecast the biological activity of compounds.
- Virtual Screening: Filtering millions of chemical structures computationally to select promising drug-like candidates.
- Experimental Validation: Labelling to support the claimed activity of compounds: VHDL Lab Testing.

- Lead Compound Identification: This entails the screening of compounds that show the labelled biological activity for further development.

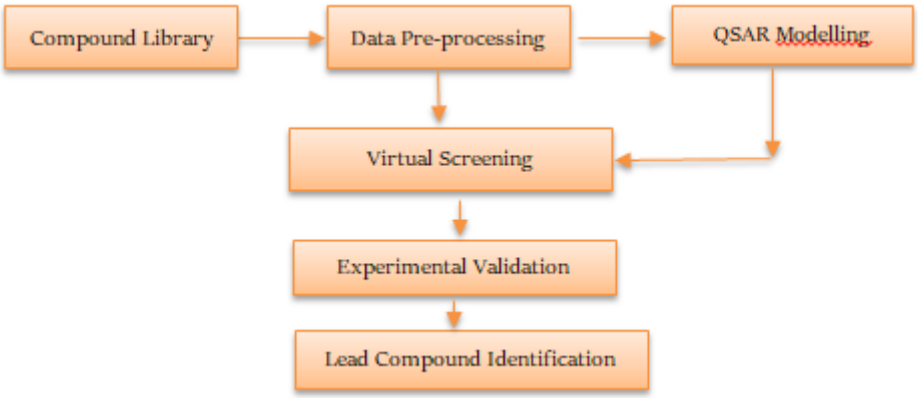

Figure 2: ML in Lead Discovery Workflow

c) Drug Design

Using design tools and AI, scientists are able to set up molecular structures to be the most effective with minimal side effects. That is how, for instance, generative models, including GANs, contributes to the development of new compounds with the required characteristics.AI in Drug Design Workflow is shown in the figure 3.

i) Techniques

1. Generative Adversarial Networks (GANs): Like any other deep learning system, GANs can create new molecular structures by learning from the inputs fed into them.
2. Molecular Docking Simulations: AI draws possible conformation of compound molecules and how they will behave with biological target; it increases the efficiency of drug discovery.

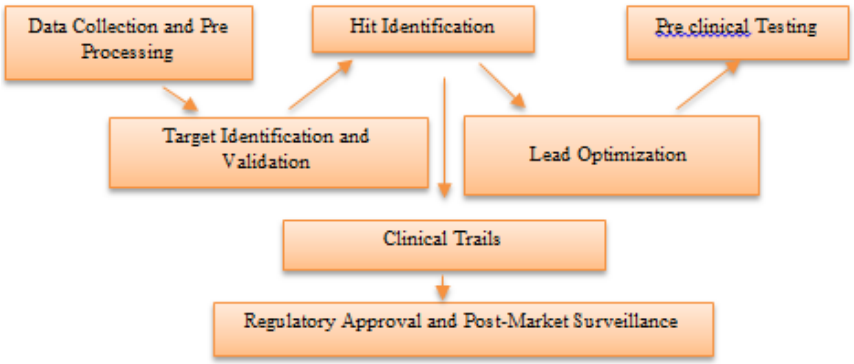

Figure 3: AI in Drug Design Workflow

d) Drug Repurposing

Rich data from AI can help to understand new applications for existing medications, thus accelerating the introduction of therapeutic agents into public circulation. [2] They can also come up with new uses of drugs that are already in the market but heard of by clinicians and other health care providers.

i) Techniques

- Data Mining: AI techniques automate the process of analysing historical clinical records to find possible new uses for the authorized medicines.
- Network Analysis: Bioinformatics BI investigate biological networks to discover fresh targets for drugs.

The outlined seven key stages are a logical and coherent approach to organizing jobs in the AI-driven drug design workflow.

i) Data Collection and Pre-processing

- Sources: Indications, Biological databases, bibliographical data, clinical trials.
- Pre-processing: Before feeding the data into the ANN, data cleaning was done to remove any missing and erroneous data with the data normalized and augmented.

ii) Target Identification and Validation

- Techniques: Genomics, proteomics, bioinformatics.

- AI Role: Application of machine learning techniques to predicting potential targets for drug molecules.

iii) Hit Identification

- Methods: Screening using many samples at a time or screenings of Computer aided simulation.
- AI Role: Employing deep learning models to quantify SAR and screen compounds according to the likelihood of forming productive interactions.

iv) Lead Optimization

- Processes: Structure-activity relationship (SAR) analysis, pharmacokinetics optimization.
- AI Role: Generation of new molecules and molecular structures with specified features and characteristics.

v) Preclinical Testing

- Tests: In vitro tests to determine the effectiveness of repurposed drugs when exposed to the virus; in vivo tests to determine the toxicity of the drugs when administered in the body.
- AI Role: ADMET and toxicity predictions using various type and level of toxicity models.

vi) Clinical Trials

- Phases: Clinical trials conducted in phases I, II and III, to establish the safety and effectiveness of a product on human candidates.
- AI Role: Since stratification of patients, idealization of trial designs and outcomes predictions constitute a core component of fulfilling demands for mHealth apps.

vii) Regulatory Approval and Post-Market Surveillance

- Approval: Reporting of data to the administrative authorities (for instance, FDA, EMA, etc.).
- AI Role: Data mining for facilitating the preparation of documents for submission to regulatory agencies and identification of adverse effects of drugs after they have been released to the market.

C. AI in Drug Repurposing Workflow

AI in Drug Repurposing Workflow and the working process are mentioned below figure 4.

a) Data Collection: The process of collecting clinical information, preclinical data, patient information, and existing information about drugs.

b) Data Integration: The process of assembling the pool of materials from different heterogeneous data sources into a single list of documents.

c) Feature Extraction: After integration of data about existing drugs and possible diseases which have n number of symptoms corresponding to the molecule, I would have filtered the probable features that could point out new uses of the old drugs.

d) Machine Learning Models: To train up the models to consider and discover other possible novel therapeutic applications from the features.

e) Prediction and Validation: Designing probabilistic forecasts on new applications and subsequent cross verification through experimental as well as clinical analysis.

f) Clinical Trials: Engaging clinical trials to establish the ascertained novel therapeutic use.

g) Drug Repurposing: To approve the drug for the new indication as well as to present and advertise the drug for that use.

D. Data Quality

Data Quality Improvement Process and the working process are mentioned below figure 5.

It also deserves of mention in this regard that it must be borne or appreciated that the quality of the models used in AI depends on the extent of such data feeds received. It implies that there can be non-perfect completion and synchronisation of input data means that the reliability of the outcomes predicted is tainted.

a) Starts

Begin the collection of actual data to complete the eradication of deficiency in the particular pharmaceutical study.

b) Data Collection

In total, buy diverse types of data that would be important for the drug discovery process, for instance, clinical, molecular data.

c) Data Cleaning

Implement AI algorithms to elevate data quality, arriving data sets for examination need preprocessing alteration.

d) Data Validation

This will require checking that the cleaned data is reliable and suitable for AI usage, as well as in the right format for analysis and modelling.

e) Data Integration

The second approach entails aggregating passed-through, augmented source databases whose information can be used to create datasets that are informative of AI and ML models.

f) End

The last step in this process to improve the current view and productiveness in drug discovery by enhancing data quality.

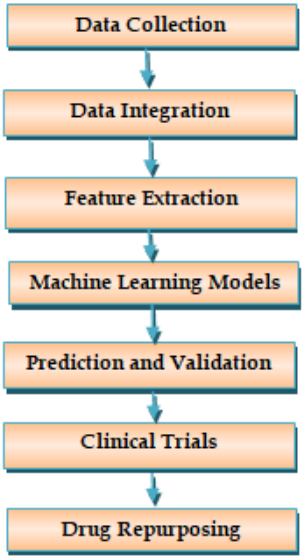

Figure 4: AI in Drug Repurposing Workflow

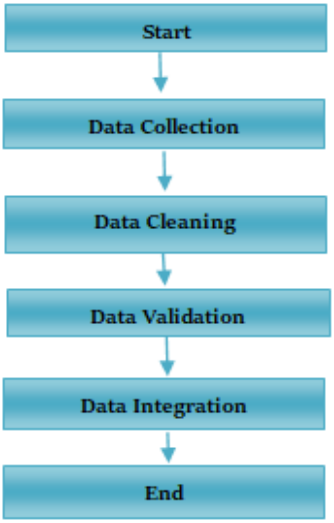

Figure 5: Data Quality Improvement Process

E. Model Interpretability

The challenge that is prevalent and affects most of the deep learning AI model is that the models are often considered as “black boxes” hence people cannot understand why a specific option has been predicted. [7] Another area where further work needs to be done is making the model more transparent in order to obtain such trust from other scientists.

F. Ethical Considerations

The modern application of artificial intelligence to enable drug discovery come out with great societal issues concerning data privacy and algorithmic bias. Bias should also not be a characteristic in artificial intelligence models in health care since they may also reflect current biases.

Table 1: Ethical Considerations in AI-Driven Drug Discovery

Issue	Description
Data Privacy	Ensuring patient data is anonymized and protected
Algorithmic Bias	Preventing bias in AI models that could affect treatment efficacy
Transparency	Making AI models transparent and interpretable

III. METHODOLOGY

A. Data Collection and Pre-processing

In the case of emerging AI and ML applications in drug discovery, data is the primary constituent. This section provides more detailed understanding of the sources, types, and the pre-treatment of data for the development of powerful AI models.

a) Data Sources and Types

i) Genomic Data:

- Description: It refers to the sequences, expression, and mutations of size and shape of genes and DNA molecules.
- Source: GenBank, Encode and the 1000 Genomes Project population-frequency databases are some examples of public databanks.

ii) Example:

- Data based on human genome chromosome studies.
- RNA-sequence gene expression data indices.

b) Chemical Structures:

- Description: Structural models: the simplified models of chemical structures that illustrate two-dimensional and three-dimensional arrangements of the molecular compounds.
- Source: Besides PubChem, chembland Zinc databases are also important.

i) Example:

- Descriptive representations of chemical compounds recorded in the form of SMILES notations.
- Molecular insights from X-ray crystallography structures to build the 3D models.

c) Biological Activity Data:

- Description: Data concerning the pharmacological profiles of compounds or modes of how they link with more specific biological receptors.
- Source: Some of the reliable database sources include, BindingDB, DrugBank and Protein Data Bank-PDB.

i) Example:

- Binding of drugs with their targets.
- Enzyme inhibition data.

d) Clinical Trial Results:

- Description: Information from preliminary randomized controlled trials that investigate safety and efficacy of drugs.
- Source: European Clinical Trials Database.

i) Example:

- Mortality and morbidity of patients and treatments from Phase III studies.
- Adverse event reports.

B. Data Pre-processing Steps

a) Data Cleaning

i. Description: Since the features dimension was significantly reduced, some cleaning of data which involves deletion of twinned elements, incorrect entries and filling of missing values.
ii. Techniques: Imputation, handling of outliers, and degassing or removal of noise are some of the methods of dealing with missing data.
iii. Example: Albeit in rare occurrences, there may be examples where a gene expression dataset will contain some missing data and these need to be handled effectively.

b) Normalization

i. Description: Normalization of them to ensure that all of the features are in the same units as those of their counterparts.

ii. Techniques: Minimum-maximum adjustment, standardization.
iii. Example: Normalizing molecular descriptors for machine learning models.

c) Feature Engineering

i. Description: Modifying the columns, including those new or combining or expanding the existing ones in a way by making them fit the pattern of data.
ii. Techniques: Practical use, concept and fundamental properties of polynomials, selecting features and reducing dimensionality.
iii. Example: Extracting fresh features from chemical structures with the help of toxicity prediction.

d) Data Splitting

i. Description: Dividing the data set into two groups in such a way that one part would be employed to obtain estimates to make the model accurate and the other part to determine how efficient the model is.
ii. Techniques: One way is a random split of the data, the other is a stratified split that divides the dataset according to classes, and the third one is an alphabetical splitting of the data.
iii. Example: Map of drug responses splitting was done into 80% for training data and only 20% for testing.

e) Data Pre-processing Workflow

Data Pre-processing Workflow and the process are mentioned below figure 6.

i) Data Collection:

- Sources: Collect the primary information from available public genomic databases, chemical databases, biological activity databases, and the index of the clinical trial results.
- Examples: For the genomic data, were used and for chemical structure data, PubChem data base were utilized for biological activity data were obtained from the BindingDB data.

ii) Data Cleaning:

- Tasks: For the cleansing of the data set an operation to remove any duplicates, erroneous values or provide for cases of missing values needs to be accomplished.
- Techniques: Imputations for missing values, deletion of outliers and cases simplifying the errors.
- Outcome: More systematic data with reduced opportunities for mistakes as far as the data input is concerned especially in cases errors such as omission of data.

iii) Normalization:

- Tasks: Meaningful scaling of data in equal proportion is defined whereby achievement of such scaling is done as to bring uniformity in the scale for a given feature.
- Techniques: Probability distribution techniques are as follows: Some other pre-processing techniques: min-max scaling, z-score normalization, etc.
- Outcome: Precise base data, that the base data can be matched and used without any change in the flow as input data for an application of machine learning.

iv) Feature Engineering:

- Tasks: If fresh samples cannot be acquired, new features need to be derived, or existing ones have been altered to uncover such patterns.
- Techniques: Polynomial representations, how to selectively retain specific features and how to eliminate unnecessary features.
- Outcome: As it turned out to build on data representation that makes a better difference in the model.

v) Data Splitting:

- Tasks: Divide the list of entries into training and control lists, as well as identify the advantages and disadvantages of the selected breakdown.
- Techniques: This is a method that entails splitting the data in a haphazard manner to get two or more segmented sets or splitting the data on the aspects of importance.
- Outcome: In such a type of situation, different set can be used with which the model can be trained and the set that will provide check when the model is validated to confirm it has not been trained with specific data that it will again find.

vi) Integration:

- Tasks: This means that it should accept the data collected by other data sources as a connected database.

- Techniques: Concatenating what must be two or more datasets with an expectation that one would get better commonality out of it.
- Outcome: A unified dataset that integrates multiple data types, ready for AI/ML model development.

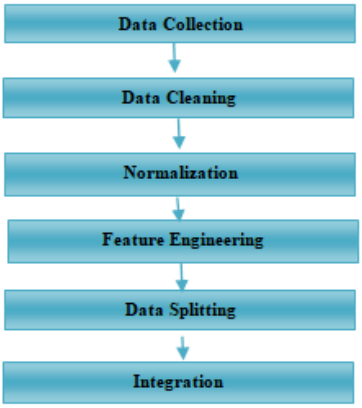

Figure 6: Data Pre-processing Process

C. Machine Learning Techniques

a) Supervised Learning

i. Classification: This is the first step in identifying molecules by their properties. For example, you can use this to determine the mutagenicity of a molecule based on its structure or gene expression profile.
Process: Take labelled datasets that have columns for features (e.g. molecular descriptors) and class labels (active/inactive) and feed into a classifier (e.g., Random Forest).

ii. Regression: The central idea of this process is to predict the data that will result from the actions of the compounds.
Process: Look at datasets where the dependent variable is the number of the potion and the rest are numeric value or level (e.g., IC50 values for drug activity) and all the regressions (e.g., LinearRegression, Neural Networks) you will create with the help of these input features will be used to predict these quantities.

iii. Applications: Anticipating the functions of biologicalactivities, toxicity, and pharmacokinetics of compounds.

iv. Models: Linear regression, decisiontrees, , neural networks, support vector machines.

v. Example: Modelling the inhibitory effect by molecular properties of a given class of drugs on a target protein employing the linear regression approach.

b) Unsupervised Learning

i. Clustering: This flow groups compounds into clusters based on their features without labels.
Process: Run clustering algorithms (e.g., K-means, Hierarchical Clustering) on molecules based on chemical structure or biological activity profiles.

ii. Dimensionality Reduction: This reduces the number of variables (dimensions) in the dataset while keeping the important information, for visualization and analysis.
Process: Use PCA or t-SNE to transform high-dimensional data into a lower dimensional space, keeping the relationships between molecules.

iii. Models: k-means, hierarchical clustering, PCA.

iv. Example: Clustering molecules by structure.

c) Unsupervised Learning

Reinforcement Learning

i. Optimization: In drug discovery, reinforcement learning can be used to optimize the molecular structures or single pair drug to get the desired properties.
    a. Process: Draw out an iterative process through which the agent (e.g., algorithmic model) produces potential drug candidates, judges their sufficiency with the use of the established criteria (e.g.,Efficiency, safety), and takes corrective actions based on feedback to make new versions delivering the maximum results (e.g., the most potent drug).

ii. Applications: Iterating feedback loops to optimize drug design.

iii. Models: Q-learning, policy gradient methods, deep Q-networks.

iv. Example: Using reinforcement learning to redesign a molecule in a designed mode where it will be more efficient and less toxic.

D. Deep Learning Models

Although deep learning is very useful in the domain of drug discovery, more specifically it helps to analyse large values of this data. This section of the paper aims at highlighting some of the crucial architectures in the deep learning field and the impact areas where they may be useful to operate at their best[10].

a) Convolutional Neural Network (CNNs)

Convolutional neural network and the process are mentioned below figure 7.

i. Applications: CNNs are beneficial for unaligned field data or partitions, application in spatial data analysis and structures of molecules and protein.
ii. Strengths: They are apt in feature extraction from images and structure data in form of tables and even Excel sheets.
iii. Example Application: In silico prediction of binding free energy of protein-ligand complexes from the structural information by CNNs.

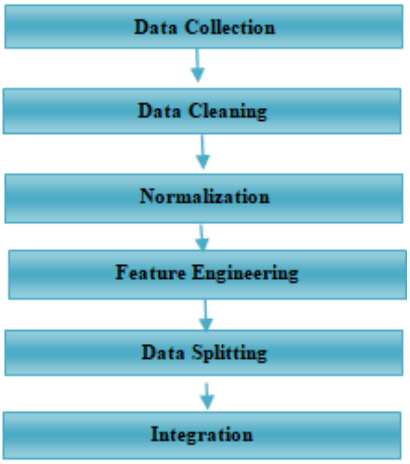

Figure 7: Convolutional neural network

- Input Layer: For inputs, the raw data, which may be molecular images or 3D structural information, is represented.
- Convolutional Layers: Late layers used for feature detection while earlier layers perform feature extraction. Every layer computes convolution operation to identify two-dimensional patterns that might be existent in the inputs.
- Activation Functions: Where, generally used with a non-linear function named as ReLU (Rectified Linear Unit) after convolution function is applied.
- Pooling Layers: As a result, scale down the feature maps which obtained to lower the dimensionality and computational power usage.
- Fully Connected Layers: These layers combine all neurons of one layer to all neurons of the next;it is used for classification or regression tasks.
- Output Layer: Gives the last prediction that could be the point of interaction between protein and ligand, or the type of physical and chemical characteristics of the molecules.

B. Recurrent Neural Networks

Recurrent Neural Networks and the process are mentioned below figure 8.

i. Applications: They can be used for analysing sequential information like genomic and protein sequences and as a result, RNNs are appropriate at analysing such sequences.
ii. Strengths: They incorporate temporal dependencies into data which are mandatory knowledge of sequences.
iii. Example Application: Challenges of using recurrent neural networks in predict critical care medicine: Time series analysis for predicting the consequences of gene mutations for protein activity.

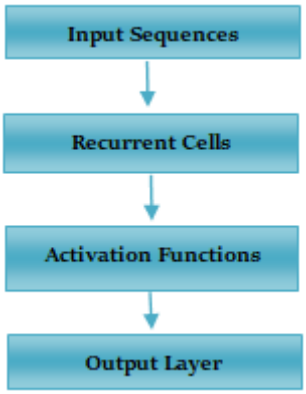

Figure 8: Recurrent Neural Networks

Components to Include:

- Input Sequences: One of the characteristics where one element comes after the other, for example, sequences of nucleotides in DNA or time-stamped events.
- Recurrent Cells (e. g., LSTM or GRU): Components within the RNN which take sequences as input and have memory of previous inputs in a network.
- Activation Functions: Usually utilized within each recurrent cell to inject non-linearity into the operation.
- Output Layer: Gives the final forecast or result for the sequential information after some processing is done on it.

c) Generative Adversarial Networks (GANs)

i. Applications: In GANs the generative models are sequential to generate new structures of a molecule endowed with the designed characteristics.
ii. Strengths: On the one hand, they create appropriate datasets with the needed realism and, on the other hand, look for new molecules in the chemical space.
iii. Example Application: The compound structures produced using GANs can be developed to have unique scaffolds that enforce required biological and chemical characteristics.

E. Natural Language Processing (NLP)

They are involved in the complex data mining as the tool for organizing and extracting information form terabytes of a textual data, [4] frequently met in scientific publications and patents.

i. Applications: Using keywords to look for medicine leads, treating drug interaction, and finding remedies.
ii. Models: Conversation mode A: One model for both speakers, multiple speakers: Transformer-based models such as BERT, NER, text classification models.
iii. Example: Text mining of theoretical material for identifying possible interaction pairs based on the use of NLP methods.

F. Model Evaluation

Objective evaluation of the AI models helps to guarantee suitability and efficiency of these models to be used in AI systems. This section describes the critical assessment and validation of measures.

a) Performance Metrics

i. Accuracy: True positive fraction: The proportion of true positive outcomes to all positives identified by a certain diagnostic process.

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

Use Case Example: The preference from poorly predicting for drug-target interactions.

ii. Precision: The ability of the model summed up the number of accurate positive cases from the total number of positive cases that the model called on.

$$Precision = \frac{TP}{TP + FP}$$

iii. Recall: It is concerned with the proportion of the total quantity of the positive observations in the actual class that was accurately predicted by the model.

$$Recall = \frac{TP}{TP + FN}$$

Use Case Example: Achieving high precision—the active compounds of a chemical can be narrowed down to minimize the exclusion of compounds while maximizing recall—toxic compounds may be difficult to determine but all possible toxic compounds must be gauged.

iv. F1-Score: How to manipulate the precision and recall statistics proportional to provide the value for the false positive as well as false negatives.

$$F1 - Score = 2 * \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

Use Case Example: Measurements for evaluating the performance of the toxicity prediction model in general terms.

v. ROC Curve and AUC: Some of the most common metrics are Area Under the Receiver Operating Characteristic (ROC) Curve and other performance measures for different classification thresholds.

b) Cross-Validation

i. Purpose: To converge the model to the minimum so that it can be tested whether it would produce good results on unseen data.
ii. Methods: k-cross validation, cross-validation, leave one out cross-validation, another one is the stratified cross validation.
iii. Example: Applying 10-fold cross validation to assess the efficacy of models predicting drug's efficacy

G. Integration with Big Data Analytics

The utilization of big data analytics platforms in association with integrated AI models is also inevitable for handling such data in pharmaceutical research.[9]

i. Platforms: Some of the leading big data frameworks and platforms are Apache Hadoop, Apache Spark, and cloud services like Amazon AWS, Google Cloud.
ii. Benefits: What are the key capabilities associated with big data applications: The three key capabilities that are often mentioned are scalability, real-time data processing, and ability to handle various types of data.
iii. Example: Implementing a real time genomics data analysis using a deep learning model combined with a SPARK based computational platform.

IV. RESULTS AND DISCUSSION

A. Advancements in AI-Driven Drug Discovery

AI and machine learning has come a long way in the drug [8] development arm of pharma and biotech industry
Recent advancements in AI and ML have led to significant breakthroughs in drug discovery:

a) Faster Target Identification: Frameworks based on artificial intelligence have helped in the prioritization of drug targets with the help of genomic and proteomic data.
b) Improved Lead Discovery: ML models have considerably decreased the time and resources required for lead discovery as the compounds' activity can be predicted with high accuracy.
c) Optimized Drug Design: AI in design tools has been employed in the creation of optimal molecular structures which improve on the effectiveness and safety of new drugs.
d) Successful Drug Repurposing: AI has also helped in finding new therapeutic uses of existing drugs so that there is new development timeline.

B. Case Studies

a) BenevolentAI

BenevolentAI applied its AI capability and utilised it to discover a solution for the curing of Amyotrophic Lateral Sclerosis (ALS). [3] The potential of baricitinib as an existing drug was discovered by their powerful AI platform when after sifting through large datasets of biomedical data.Table 2

Table 2: BenevolentAI Case Study

Aspect	Description
Disease Targeted	ALS
AI Technique	Data mining and pattern recognition in biomedical data
Outcome	Identification of baricitinib as a potential treatment

b) Atomwise

The application of deep learning helped in identifying inhibitors for the Ebola virus through Atomwise. Their AI platform called AtomNet, leveraged convolutional neural networks in learning molecular structures and biological activities table 3.

Table 3: AtomwiseCase Study

Aspect	Description
Disease Targeted	Ebola
AI Technique	Convolutional neural networks for structure-based drug design
Outcome	Identification of promising inhibitors for the Ebola virus

C. Comparative Analysis

The following is a comparison of the traditional and the AI approaches, which shows the benefits of using AI:

i. Efficiency: By using the various techniques of machine learning, AI models have the capacity to analyse big data and save the time needed to discover drugs.
ii. Cost-Effectiveness: Thus, with the application of AI, a company can minimize the costs of late-stage failures because the system unfailingly determines which drug candidates will be successful.
iii. Precision: Since AI-based models are better to learn the intricate patterns within data, the treatments are innovative and targeted than traditional methods.

D. Challenges and Future Directions

i. Data Quality and Availability: Acquiring accurate, comprehensive big data is a key requirement when constructing an AI system.
ii. Interpretability: There is a need to increase the transparency of AI models so that the scientific community and the regulatory authorities can put their trust in AI.
iii. Ethical and Regulatory Considerations: Mitigating the ethical issues and setting the legal norms on how AI can and should be used in the development of new medication will be some of the aspects that will need to be firmly defined to ensure the large-scale application of the technology.

V. CONCLUSION

Among the disruptive technologies that are expected to transform drug discovery in the coming years include AI and ML since they promise to add value to the process, decrease costs and increase the rate of success in new therapeutic agents. However, further improvements have been made, it is crucial to precede constant cooperation of computational scientists, biologists and regulations bodies to step forward to great possibilities of these technologies. Considering such difficulties as improving the quality of the input data, explaining the results produced by artificial intelligence, and dealing with ethical issues, AI for drug discovery may unlock the opportunities for further development of precise approaches in the field of pharma.

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