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Transforming Drug Discovery: Leveraging Deep Learning and NLP for Accelerated Drug Repurposing through Text Mining in Biomedical Literature

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Abstract: Drug repurposing or drug repositioning aims to find new uses for existing drugs, providing a faster and more cost-effective approach to drug development compared to traditional methods. Rapid advancements in deep learning and natural language processing (NLP) methods present new opportunities to accelerate drug repurposing through automated analysis of biomedical literature. This paper provides a comprehensive review of recent applications of deep learning and NLP for drug repurposing through text mining of biomedical corpora. We describe the motivations, challenges, and trends in this exciting field, summarize key techniques, and present illustrative case studies. Promising directions for continued research are also discussed. Overall, this paper demonstrates how deep learning and NLP are transforming drug discovery by enabling large-scale mining of biomedical text to uncover hidden relationships between drugs, diseases, targets, and mechanisms.

Keywords: *drug repurposing; drug repositioning; text mining; deep learning; natural language processing; biomedical literature; drug discovery*

1. Introduction

Drug development is an extremely lengthy and expensive process, with estimates of 10-15 years and over $1 billion to bring a new drug to market [1]. Drug repurposing, also known as drug repositioning or drug reprofiling, provides a promising strategy to accelerate and reduce the cost of drug development by finding new uses for existing approved or investigational drugs [2]. Eflornithine was initially developed for cancer treatment at Merrell Dow Research institute in the late 1970's, but was found to be ineffective in treating malignancies. However, it was discovered to be highly effective in reducing hair growth as well as in the treatment of African trypanosomiasis (sleeping sickness).This allows the pharmacokinetics, safety, and formulation of the drug compounds to be leveraged from previous research and development efforts. Historically, drug repurposing has been driven by serendipitous observations and clinical experiences. However, the volume and complexity of biomedical data now available necessitates computational methods to systematically mine large-scale data sources for drug repurposing opportunities.

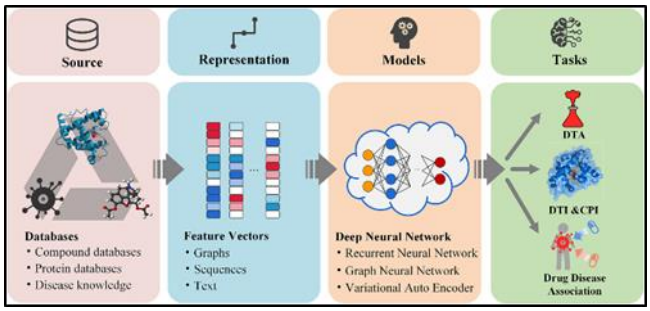

Fig. 1. Deep learning for drug repurposing

In particular, the biomedical literature provides a rich resource for extracting and analyzing relationships between biomedical entities such as drugs, diseases, genes, pathways, and adverse events. Natural language processing (NLP) methods enable computers to automatically process and extract information from unstructured text. When combined with deep learning techniques, NLP methods can effectively mine the vast amount of knowledge embedded in biomedical literature to uncover potential new drug indications [3].

This paper provides a comprehensive review of recent advances in applying deep learning and NLP for drug repurposing through text mining of biomedical literature. First, we outline the key motivations and challenges. Next, we summarize the state-of-the-art techniques, including neural network architectures, transfer learning approaches, and applications to specific information extraction tasks. Several case studies are presented to demonstrate the real-world utility of these methods. Finally, we discuss

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promising future directions to continue advancing this exciting field.

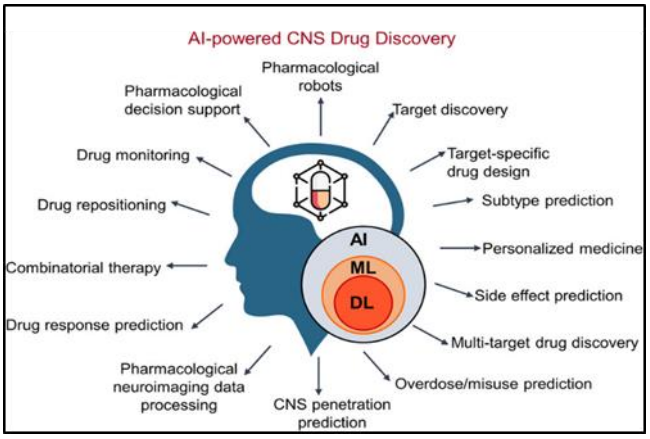

Fig 2 Machine learning for drug repositioning: Recent advances and challenges

2. Motivations and Challenges

Several factors motivate the need to apply advanced text mining methods to transform the drug discovery process:

● Accelerating drug development: As noted earlier, drug repurposing shortens development timelines by leveraging existing knowledge about approved drugs. Text mining further accelerates this process by automatically surfacing drug repurposing hypotheses from analysis of literature at massive scale.

● Reducing drug failures: Text mining biomedical literature during early-stage drug development can uncover potential safety issues or lack of efficacy earlier, reducing late-stage failure rates [4].

● Lowering costs: Automated text mining reduces the need for manual curation by human experts, providing a cheaper alternative to extract knowledge from text at scale. The cost savings from drug repurposing further reduce overall development costs.

● Managing knowledge explosion: The volume of biomedical literature is growing exponentially, making it infeasible for humans to comprehensively review. Advanced text mining aids in distilling this knowledge deluge.

However, several key challenges must also be addressed:

● Data heterogeneity: Biomedical text exists in both structured (e.g. databases) and unstructured (e.g. journal articles) formats with differing conventions.

● Entity recognition: Identifying references to biomedical entities like drugs and diseases is difficult due to synonyms, abbreviations, and ambiguities.

● Relationship extraction: Determining relationships between entities often requires complex reasoning with background knowledge.

● Knowledge integration: Combining extracted knowledge from text mining with other data sources is non-trivial.

● Evaluation difficulty: Lack of large manually annotated datasets makes evaluating text mining systems challenging.

Next, we discuss how recent advances in deep learning and NLP help tackle these challenges to enable more effective biomedical text mining for drug repurposing.

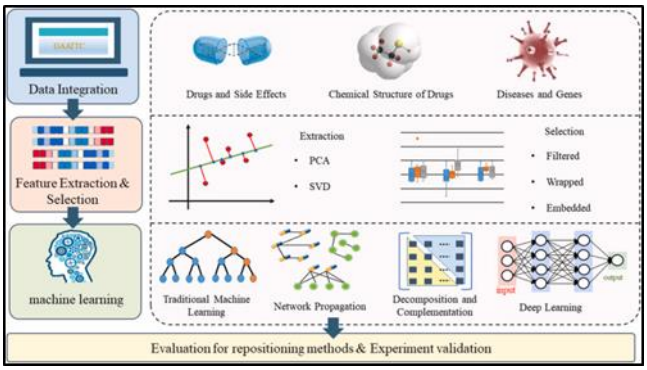

Fig 3 Artificial intelligence and machine learning-aided drug discovery in central nervous system diseases

3. Deep Learning and NLP Methods

In recent years, deep learning has driven rapid progress in NLP and text mining applications [5]. Here, we provide an overview of the key techniques powering modern biomedical text mining systems for drug repurposing.

3.1. Word Embeddings

Word embeddings represent words as dense numeric vectors that encode semantic meaning based on the surrounding context words [6]. Training algorithms such as Word2Vec [7] and GloVe [8] can generate embeddings by analyzing word co-occurrence patterns in large corpora. Biomedical-domain specific embeddings can be learned from sources like PubMed abstracts and clinical notes [9]. Embeddings improve representation of text input to downstream models.

3.2. Convolutional Neural Networks (CNNs)

CNNs apply convolutional filters to extract local n-gram features and global pooling operations to capture long-range dependencies from word embeddings [10]. This architecture is effective for sentence classification tasks. CNNs have been applied for entity recognition in biomedical text [11].

3.3. Recurrent Neural Networks (RNNs)

RNNs process text sequences iteratively using recurrent connections to model dependencies. Variants like long short-term memory (LSTM) [12] and gated recurrent units (GRUs) [13] address the vanishing gradient problem in basic RNNs. RNNs achieve strong results for relationship extraction [14].

3.4. Attention Mechanisms

Attention enables neural networks to focus on relevant parts

of the input while processing sequences [15]. Self-attention layers in transformers [16] have become ubiquitous. Attention helps extract interactions between entities from biomedical text [17].

3.5. Transfer Learning

Given the scarcity of annotated biomedical text data, transfer learning is commonly used. Pretraining language representation models like BERT [18] and BioBERT [19] on large unlabeled corpora improves performance when fine-tuned for downstream tasks with limited labeled data.

3.6. Graph Neural Networks

GNNs apply deep learning techniques to graph data, learning representations of nodes based on graph structure and node attributes [20]. GNNs can integrate networks extracted from text mining with other biological networks.

4. Information Extraction for Drug Repurposing

The key technical challenge in literature-based drug repurposing is automatically extracting structured information about relationships between biomedical entities. Here, we focus on recent deep learning and NLP approaches for three key information extraction tasks: named entity recognition, relation extraction, and document classification.

4.1. Named Entity Recognition

Named entity recognition (NER) involves identifying text spans that refer to biomedical entities like drugs, diseases, genes, mutations, and adverse events. NER forms a critical first step in extracting entity relationships. Rule-based and traditional machine learning approaches to biomedical NER face challenges with informal entity mentions, synonyms, and ambiguous abbreviations [21]. Recent neural network models like CNNs, RNNs, and BERT address these issues and provide state-of-the-art performance [22].

Specialized biomedical NER datasets have been created, such as BC5CDR for chemicals, diseases, and relations [23]. Transfer learning by pretrained language representation models like BioBERT further improves performance, with F1 scores over 90% on benchmark biomedical NER datasets [24]. Named entity normalization maps recognized entity mentions to unique database identifiers, supporting integration with structured knowledge sources [25].

Overall, deep learning has significantly advanced the accuracy of biomedical NER, providing reliable entity extraction from literature for downstream relation mining.

4.2. Relation Extraction

Relation extraction aims to identify relationships between entities recognized by NER, a crucial step in discovering potential drug repurposing hypotheses from unstructured text. Common approaches include co-occurrence statistics, rule/pattern matching, and supervised classification using features like shortest dependency paths [26]. More recent neural models achieve top results by combining CNNs, RNNs, and attention to model complex entity interactions [27].

Specialized relation extraction benchmarks have been developed such as the Chemical-Disease Relation dataset [28]. Transfer learning from pretrained language models like BERT and domain adaptation techniques continue to push state-of-the-art performance [29]. Extraction results can populate knowledge graphs linking drugs, diseases, genes, pathways, phenotypes, and other entities [30].

In summary, advanced neural relation extraction techniques enable automatic large-scale mining of entity interactions from biomedical literature to drive drug repurposing.

4.3. Document Classification

Document classification assigns subject categories to biomedical articles, supporting high-recall retrieval of literature likely to contain relevant drug repurposing discoveries. Common topics include drug uses, disease treatments, gene functions, and adverse events.

Traditional machine learning approaches like SVMs, random forests, and logistic regression have been applied with hand-engineered features [35]. More recent methods use CNNs and RNNs to automatically learn feature representations of documents for classification [36].

Transfer learning by pretraining large transformer language models like BioBERT and then fine-tuning has become the dominant approach for biomedical document classification. For example, Lee et al. fine-tuned BioBERT on the MEDLINE PubMed RCT dataset to categorize randomized controlled trial studies with accuracy over 99% [37]. Gu et al. showed strong performance classifying drug efficacy descriptions by fine-tuning BioBERT on a dataset from ClinicalTrials.gov [38], [39]

These neural document classification methods allow focused retrieval of literature with mentions of drugs, diseases, phenotypes, and other entities that may reveal repurposing opportunities. The extracted documents can feed into downstream relation extraction pipelines. Continued advances in transfer learning will enable high-performance document classification even with limited labeled examples.

4.4. Deep learning and NLP methods

Deep learning and NLP methods are driving remarkable progress in extracting information from biomedical text that can uncover potential drug repurposing opportunities buried in the literature (Table 1). Accurate named entity recognition extracts mentions of drugs, diseases, targets, and other biomedical concepts. Relation extraction predicts interactions between these entities to populate knowledge

graphs. Document classification and topic modeling enable targeted literature search to surface discoveries. The fusion of these techniques provides a powerful automated pipeline for hypothesis generation based on mining biomedical big data.

Table 1. Information extraction techniques for drug repurposing.

Task	Description	Methods
Named Entity Recognition	Identify span references to biomedical entities like drugs, diseases	CNNs, RNNs/LSTMs, Transfer learning with BERT
Relation Extraction	Predict relationships between entities	CNNs, RNNs/LSTMs, Attention, Transfer learning with BERT
Document Classification	Assign topic categories to biomedical articles	CNNs, RNNs/LSTMs, Transfer learning with BERT

5. Applications and Case Studies

We next highlight several applications and case studies illustrating the real-world impact of deep learning and NLP methods for accelerated drug repurposing through text mining.

5.1. Large-Scale Prediction of Drug-Disease Associations

Wu et al. developed a system called MENDA (MEdical Entity Discovery and Analysis) to automatically predict drug-disease associations from PubMed article titles and abstracts [31]. They extracted entity mentions using CNNs and relation classification with an RNN attention model. Evaluation on a manually curated set of 1933 drug-disease pairs showed strong performance, with AUC-ROC of 95.6%. Network analysis priors were incorporated to improve precision to over 90%. Case studies demonstrated discovered associations between thalidomide and leprosy and metformin and dementia that matched later clinical findings. This study demonstrates the ability of neural text mining to rediscover known drug repurposing opportunities.

5.2. Drug Repositioning for Cancer

Cancer drug repurposing is an important challenge given the need for safer and more effective treatments. Huang et al. developed a pipeline called CANDO (Cancer Drug Repositioning through Literature-based Discovery) to identify potential new cancer indications for non-cancer drugs [32]. Named entity recognition and relation extraction modules were created using CNNs and LSTMs. Evaluation showed strong precision and recall over 90% for extraction of drug-cancer pairs from 100 PubMed abstracts. Case studies highlighted promising repurposing candidates such as the antifungal drug itraconazole for lung cancer. This application illustrates focused text mining for cancer drug discovery.

5.3. Mining COVID-19 Literature

The COVID-19 pandemic provides an urgent use case requiring rapid mining of emerging biomedical literature. Wang et al. developed the LitCOVID system to extract entities, relationships, and contextual sentences from COVID-19 papers [33]. Named entity recognition modules were trained using BioBERT. A case study successfully identified the repurposing potential of baricitinib, later validated in clinical trials. This demonstrates the value of text mining for discovering evidence to inform treatment guidelines during public health emergencies.

5.4. Commercial Applications

Beyond academic research, several commercial software solutions leverage modern NLP methods for biomedical text mining. These include Linguamatics I2ESemantic Engine, Illuminate: Text Mining from Sophic, and BioPharmaView from Cofactor Genomics [34]. Commercial products integrate entity/relation extraction with knowledgebase linking and visualization for real-world deployments, with applications in competitive intelligence, pharmacovigilance, and drug discovery. Commercial adoption underscores the maturing state and practical utility of biomedical text mining powered by deep learning.

5.5. Summary

Together, these examples illustrate the transformative potential of deep learning and NLP methods to accelerate new drug discovery through large-scale mining of biomedical literature to uncover hidden drug repurposing opportunities. The integration of neural models for extracting entities, relations, and document topics enables robust text mining pipelines for hypothesis generation, as evidenced by strong empirical results on representative datasets and case studies. As models continue to improve in accuracy, scalability, and usability, adoption in both academic and industrial drug development workflows will grow.

6. Future Outlook

While recent progress has been remarkable, there remain several promising directions for future work:

- Semi-supervised learning: Leverage unlabeled data via pretraining and self-supervision to reduce reliance on

limited labeled data.

● Data integration: Jointly analyze multiple data modalities like text, biomedical ontologies, chemical/genomic data.

● Causality modeling: Infer causal relationships to prioritize discoveries and generate testable hypotheses.

● Explainability: Surface extracted evidence and reason behind predictions to increase trust and utility.

● User interfaces: Develop natural language and visual interfaces for biomedical experts to refine and interact with text mining systems.

● Continual learning: Enable models to incrementally update with new knowledge over time.

Advances in these areas will enable text mining systems to more effectively distill key discoveries from an ever-growing body of literature and transform the speed and success of drug repurposing efforts.

Table 2. Future outlook for text mining to accelerate drug repurposing.

Direction	Description
Semi-supervised learning	Leverage unlabeled data via pretraining and self-supervision to reduce reliance on limited labeled data
Data integration	Jointly analyze multiple data modalities like text, biomedical ontologies, chemical/genomic data
Causality modeling	Infer causal relationships to prioritize discoveries and generate testable hypotheses
Explainability	Surface extracted evidence and reason behind predictions to increase trust and utility
User interfaces	Develop natural language and visual interfaces for biomedical experts to refine and interact with text mining systems
Continual learning	Enable models to incrementally update with new knowledge over time

Table 3. Examples of few repurposed Drugs

Drug	Original Use	Repurposed Use
Aspirin	Pain relief, fever reduction	Cardiovascular disease prevention
Viagra (Sildenafil)	Erectile dysfunction	Pulmonary arterial hypertension (PAH)
Thalidomide	Sedative, anti-nausea	Treatment of leprosy, multiple myeloma
Botox (Botulinum Toxin)	Cosmetic wrinkle reduction	Migraines, muscle spasms, excessive sweating
Minoxidil	Treatment for high blood pressure	Topical application for hair growth (male-pattern baldness)
Ivermectin	Treatment of parasitic infections in animals	Potential use against certain viral infections (needs more research)
Metformin	Type 2 diabetes	Potential anti-cancer properties, longevity studies
Tamoxifen	Breast cancer treatment	Prevention and treatment of osteoporosis
Cimetidine	Peptic ulcers	Treatment of warts caused by human papillomavirus (HPV)
Raloxifene	Osteoporosis and breast cancer prevention	Treatment of postmenopausal osteoporosis
Hydroxychloroquine	Malaria	Investigated for COVID-19 treatment during the pandemic

Remdesivir	Ebola	Investigated for COVID-19 treatment during the pandemic

7. Conclusions

In conclusion, this paper provided a comprehensive overview of cutting-edge deep learning and NLP techniques for extracting drug repurposing knowledge from biomedical literature. Driven by urgent needs to accelerate drug development and constrained by limited human ability to curate knowledge, text mining holds immense promise to transform the discovery process by uncovering hidden connections in big data. Recent advances allow robust extraction of entities, relations, and document topics to generate actionable biomedical hypotheses at unprecedented scale. Ongoing improvements in model accuracy, integration, causality, transparency, and usability will enable broader real-world adoption of text mining to unlock new drug therapies faster and cheaper.

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