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Knowledge Graph Enhanced DRL-based Personalized Medication Recommendation System

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Abstract: The fragmentation of knowledge in the pharmaceutical field, insufficient retrieval efficiency, and deviation in personalized services have long constrained the effective dissemination and clinical application of professional information. Although conventional medical recommendation systems can meet basic service needs, such systems face two major bottlenecks when integrating complex knowledge graphs in the pharmaceutical field: firstly, it is difficult to fully parse deep semantic associations in the knowledge network; Secondly, it is impossible to accurately track the dynamic evolution characteristics of user needs. In view of this, this study explores the integration of pharmaceutical knowledge resources and the improvement of recommendation accuracy from two dimensions, focusing on innovative research on efficient pharmaceutical knowledge graph construction technology and intelligent recommendation algorithm optimization based on semantic networks. The aim is to break through the technical constraints of traditional recommendation systems and build more explanatory and adaptive knowledge service solutions for the medical industry.

1. Introduction

With the deep integration of medical technology and information technology, the pharmaceutical field, as a traditional wisdom system carrying a profound theoretical system, is becoming a focus of industry attention for the systematic integration and intelligent application of knowledge. However, the specialized and systematic characteristics of knowledge in the pharmaceutical field pose significant challenges to traditional knowledge management models. Firstly, pharmaceutical knowledge spans multiple dimensions such as pharmacological mechanisms, diagnostic and therapeutic techniques, and clinical plans. Its fragmented storage state and lack of standardization make it difficult for conventional databases to achieve efficient and accurate knowledge retrieval, which restricts the dissemination efficiency of professional knowledge; Secondly, clinical practice requires a deep integration of professional knowledge with specific diagnosis and treatment scenarios, which is a complex decision-making process that cannot be supported by simple retrieval; Furthermore, in the face of the breakthrough progress of artificial intelligence technology, how to

transform cutting-edge technology into a driving force for promoting pharmaceutical knowledge innovation has become an urgent issue for the industry to break through. Against the backdrop of the booming development of the artificial intelligence industry, the integration and innovation of natural language processing technology and knowledge graph technology in deep learning have brought innovative opportunities to the industry. As an important carrier of structured knowledge representation, knowledge graphs transform dispersed medical concepts into computable knowledge units by constructing entity relationship networks. This technological architecture is particularly suitable for handling complex knowledge systems in the pharmaceutical field. Its multi-dimensional semantic description ability and logical reasoning support lay the foundation for building intelligent recommendation systems, which can improve the accuracy of knowledge services and optimize user experience. This study focuses on the knowledge management needs in the pharmaceutical field and has developed an intelligent recommendation system based on semantic networks. Through digital means, the efficiency of knowledge services has been optimized, which will contribute to the further development of personalized medication decision-making in clinical practice.

2. Construction of Knowledge Graph

2.1. Application of Knowledge Graph

Knowledge graph is a structured knowledge representation method that organizes and expresses entities, concepts, and their complex relationships through graph data structures. Its structured structure provides strong support for information retrieval, reasoning, and analysis. Here, the knowledge graph adopts a resource description framework triplet architecture to achieve the associated storage of knowledge elements in the medical field. This structured modeling approach constructs a multidimensional relationship network between modern pharmaceutical concepts through a bidirectional expression mechanism of "subject attribute value" and "subject association object". In the clinical pharmacy knowledge system, professional elements such as drug composition, indications, and mechanisms of action are defined as independent entities, each carrying multidimensional feature descriptions. Taking typical drug entities as an example, their attribute system covers characteristic parameters such as pharmacological classification, target of action, contraindications, etc; The disease entity includes structured information such as diagnostic criteria, treatment pathways, and associated medications; The administration plan entity includes more elements such as dosage specifications, suitable population, and efficacy monitoring. In the typical knowledge graph application scenarios shown in Figures 1 and 2, entities such as "aspirin", "angina pectoris", "amlodipine", and "hypertension" form a knowledge network through semantic association. Among them, "aspirin" and "angina pectoris" establish a "subject association object" triplet through a "therapeutic" relationship, while the drug and the "antipyretic and analgesic" attribute form a semantic association of "subject attribute attribute attribute value"; The entity of "hypertension" and "amlodipine" form a triplet through the relationship of "applicable drugs", while labeling the "calcium channel blocker" category attribute and "long-acting antihypertensive" characteristic value of the drug. This dual expression mechanism not only clearly characterizes the relationship between drug characteristics and treatment, but also reveals the inherent logical structure of the modern pharmaceutical knowledge system through topological connections between nodes, providing basic infrastructure support for building intelligent clinical decision support systems.

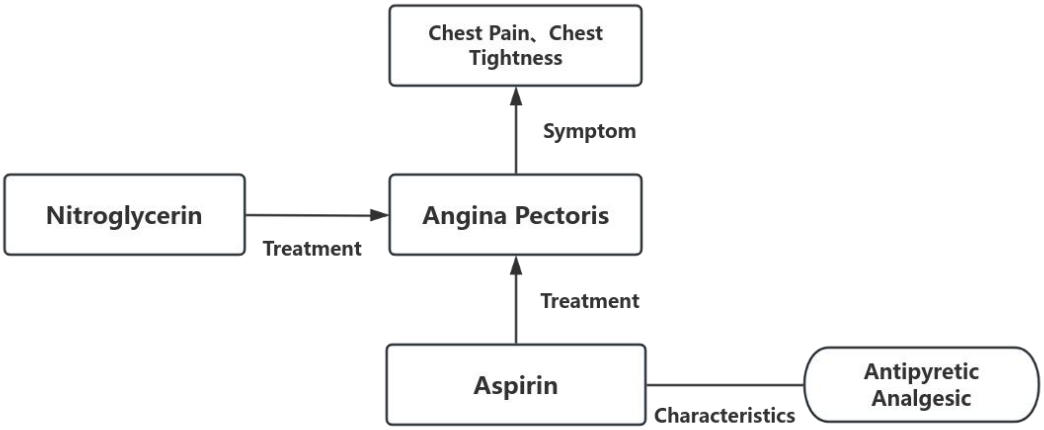

Figure 1. Angina Pectoris Knowledge Graph Example

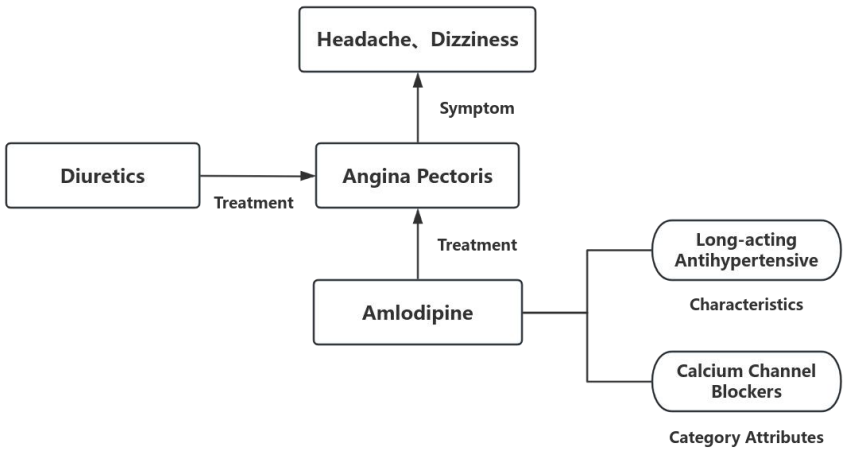

Figure 2. Hypertension Knowledge Graph Example

2.2. High order Heterogeneous Graph

In order to deeply explore the complex relationships in medical data, this study uses high-order heterogeneous graphs to represent the medical knowledge graph. The medical knowledge graph is essentially a high-order heterogeneous information network, mainly reflected in two aspects: the diversity of node types (drugs, diseases, symptoms, genes, side effects, patients, etc.) and the complexity of relationship types (treatment, cause, inhibition, interaction, belonging, applicable, etc.). This heterogeneity goes far beyond simple isomorphic graph structures, containing rich semantic information and potential higher-order correlations. In order to effectively model this complexity and capture deep semantic associations beyond direct neighbors, this study adopts a meta path guided graph neural network (GNN) framework. Meta path is defined as a sequence of node types as follows:

$$\phi = V_1 \xrightarrow{R_1} V_2 \xrightarrow{R_2} \cdots \xrightarrow{R_l} V_{l+1} \qquad (1)$$

It defines a composite relationship path between nodes with specific semantics. For example, drug disease drug: revealing drugs (potential substitute drugs or combination drugs) for treating the same disease. Drug Side Effects Drug: Revealing drugs with similar side effect profiles (warning of

potential side effect overlay risks). Patient Disease Drug Side Effects: Connect the patient's medical history, medication use, and potential risk of side effects. By predefining a set of clinically significant meta paths, the system can aggregate information from multi hop neighbors and learn context aware representations of nodes in specific semantic paths. As shown in Figure 3, around the target drug node (such as "warfarin"), the system can aggregate drug information affected by the same gene along the "drug gene drug" path (revealing metabolic interaction risks), while aggregating other drug information for treating the same disease (such as "atrial fibrillation") along the "drug disease drug" path (revealing alternative solutions). This meta path based neighborhood aggregation mechanism enables the model to understand complex and indirect medical associations, laying a semantic foundation for subsequent accurate recommendations.

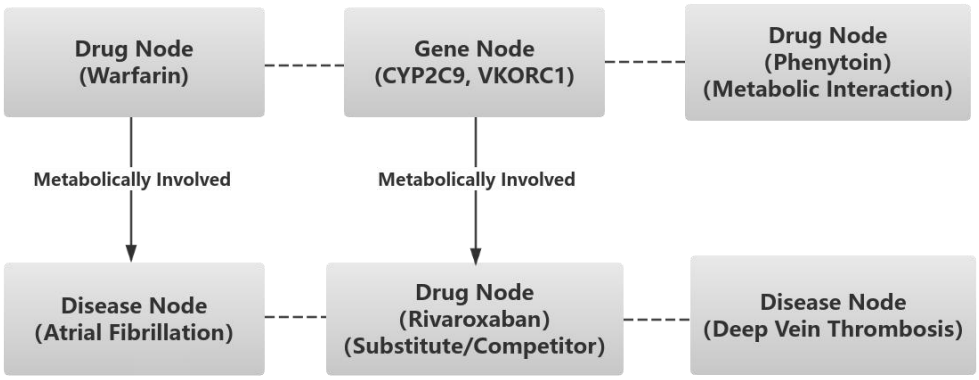

Figure 3. Meta-path Based High-order Neighborhood Aggregation Schema

2.3. Relationship Extraction

The core challenge in building a high-quality medical knowledge graph is to automatically and accurately extract structured (head entity, relationship, tail entity) triplets from massive, heterogeneous, and unstructured raw data. This system adopts a multimodal fusion and hybrid relationship extraction strategy. The data sources include: 1. Structured/Semi structured data: authoritative medical databases (such as DrugBank, PharmGKB, CTD, MeSH), drug instructions, clinical diagnosis and treatment guidelines, ICD/ATC coding libraries. These data provide high-quality core triplets, extracted through pre-defined mapping rules and patterns. 2. Unstructured textual data: electronic health records (EHRs), clinical research literature (PubMed), medical encyclopedias. These are the main sources for mining new knowledge and fine-grained relationships.

The extraction technique utilizes the following components:

1. Joint extraction based on pre trained language model (PLM): Using an architecture similar to BERT BiLSTM CRF, sequence annotation is performed on input medical text, while identifying entity boundaries and their relationship types. The model has been fine tuned on medical corpora such as MIMIC-III clinical note subsets and PubMed abstracts.

2. Rule and pattern matching: Define rules based on keywords, syntactic templates (such as [Drug] is contraindicated in [Disase]), and dictionaries for specific high-frequency, high certainty relationships (such as "Drug Contraindications", "Drug Indications") to improve the accuracy and efficiency of extraction.

3. Ontology alignment: Using medical ontologies such as UMLS, the extracted entities are semantically standardized (normalized to standard concept IDs), and relationships are semantically verified and enriched.

In order to ensure the quality and effectiveness of the knowledge graph, a multi-level quality assurance system has been developed. In the data collection stage, a multi-source verification mechanism is adopted to cross validate third-party information from multiple independent sources. When the same medical fact is repeatedly verified by authoritative sources such as drug regulatory databases and clinical diagnosis and treatment guidelines, its confidence level will be exponentially improved. A dynamic conflict resolution protocol has been developed for data conflict scenarios: when there is a conflict between electronic medical records and the latest version of drug instructions, the system automatically activates an evidence-based arbitration mechanism, giving higher priority to legally binding drug instructions; For disputes over literature of the same level, a time decay factor is introduced, and high-quality clinical studies published within the past three years are prioritized. In key medical fields such as drug interactions and contraindication identification, a closed-loop expert review process has been specially designed, and a visual verification interface has been developed to support clinical pharmacists in quickly verifying automatically extracted results. The system also records expert correction trajectories and optimizes algorithm parameters in reverse.

3. System algorithm

3.1. Graph Attention Network

In order to dynamically capture the differences in importance of different neighboring nodes to the central node in the medical knowledge graph (for example, the main indication information of a drug may be more important than the secondary pharmacokinetic parameters for current patient recommendation), and effectively fuse the high-order heterogeneous information defined in Section 2.2, the system adopts Graph Attention Network (GAT) as the core encoder. The core idea of GAT is to learn the attention weights of its neighbors for each node, achieving differentiated information aggregation. Given the set of central node i and its neighboring nodes N (i), the output features of node i at layer l are calculated as follows:

$$e_{ij}^{(l)} = \text{LeakyReLU}\left(\vec{a}^{(l)^T}\left[W^{(l)}\vec{h}_i^{(l-1)} \middle\| W^{(l)}\vec{h}_j^{(l-1)}\right]\right) \quad (2)$$

For each neighbor j∈N(i), calculate the unnormalized attention coefficient eij, where W(l) is the learnable weight matrix and a(l) is the learnable parameter vector of the single-layer feedforward neural network. Then use the softmax function to normalize eij and obtain the attention weight aij:

$$a_{ij}^{(l)} = \frac{\exp\left(e_{ij}^{(l)}\right)}{\sum_{k\in N(i)}\exp\left(e_{ij}^{(l)}\right)} \quad (3)$$

Using the learned attention weights to weight and sum the features of neighboring nodes, the aggregated representation of node i is obtained:

$$\vec{h}_i^{(l)'} = \sigma\left(\sum_{j\in N(i)}\partial_{ij}^{(l)}W^{(l)}\vec{h}_j^{(l-1)}\right) \quad (4)$$

To stabilize the learning process and capture semantic information from different subspaces, K independent attention heads are typically used for computation, and their outputs are concatenated:

$$\vec{h}_i^{(l)} = \Big\|_{k=1}^{K}\sigma\left(\sum_{j\in N(i)}\partial_{ij}^{(l,k)}W^{(l,k)}\vec{h}_j^{(l-1)}\right) \quad (5)$$

3.2. Model Framework

The overall system framework KG-DRL consists of a tightly coupled knowledge graph

embedding module and a deep reinforcement learning recommendation module. The core goal of the knowledge graph embedding module is to map diverse entities (such as drugs, diseases, patients, genes) and complex relationships in the graph to a low dimensional, continuous vector space, while preserving their inherent semantic information and structural features to the greatest extent possible. To achieve this goal, this system adopts a hybrid architecture of GAT+TransR, fully utilizing the modeling ability of graph attention networks for high-order heterogeneous neighborhoods and the characterization ability of TransR for relationship specific semantic spaces. Graph Attention Network (GAT) encoder serves as the fundamental feature extraction layer. Input the initial feature vector of the entity. The core of applying multi-layer GAT to process knowledge graphs lies in dynamically learning the importance weights between the central node and its neighboring nodes through attention mechanisms. The output of GAT, HGAT, contains high-order contextual information of entities in the graph, particularly highlighting neighboring nodes and relationship paths that are crucial for the current task through attention weights.

However, the embedding vectors learned by GAT are located in a single shared semantic space, and their discriminative ability may be insufficient for the characteristics of numerous relationship types and significant semantic differences in medical graphs. Therefore, based on GAT encoding, this system further introduces the TransR model for refinement. The core idea of TransR is to learn a specific projection space for each relationship r and optimize the scoring function of triplets (h, r, t):

$$h_{\perp} = h_{GAT}^{e} M_r \quad (6)$$

$$t_{\perp} = t_{GAT}^{e} M_r \quad (7)$$

$$f_r(h,t) = \left\| h_{\perp} + r - t_{\perp} \right\|_{L_1/L_2}^2 \quad (8)$$

The goal of model training is to minimize the score of positive triples while maximizing the score of negative triples generated through negative sampling. This process significantly enhances the model's ability to distinguish complex medical relationship semantics, especially for accurately modeling key constraint relationships such as drug interactions and contraindications.

The KG-DRL framework models personalized medication recommendation as a serialized decision optimization problem. The system simulates the clinical decision-making process through deep reinforcement learning (DRL) intelligent agents: the agent selects medication adjustment actions based on the patient's current health status, and the environment transitions to a new state according to medical logic and provides immediate rewards. The goal is to maximize long-term cumulative rewards, that is, to achieve the optimal dynamic balance between efficacy and safety. State representation accurately encodes multidimensional patient information. The state vector st integrates structured features (demographics, vital signs) with semantic entity vectors provided by the knowledge graph embedding module (current diagnostic disease, key medical history, relevant test indicators, genotype, and current medication). Integrating heterogeneous features through a multi-layer perceptron (MLP) encoder to form a compact context aware representation st '. The introduction of knowledge graph embedding enables states to contain rich medical related semantics (such as drug disease treatment relationships, gene metabolic pathways), providing deep basis for decision-making. Action space is defined as a discrete medication regimen adjustment operation, including: adding medication from a pre screened candidate set (dynamically generated based on indications and contraindications), removing current medication, adjusting dosage, or maintaining the status quo. This design conforms to the clinical decision-making granularity and ensures basic safety through knowledge graph relationship constraints. The reward function is the core engine driving strategy optimization, and its design takes into account clinical objectives:

$$r_t = r_t^{efficacy} + r_t^{safety} + r_t^{compliance}$$

Efficacy reward $r^{efficacy}$ positive correlation improvement in key indicators (such as blood pressure decrease ΔSBP, blood glucose decrease ΔHbA1c). Safety penalties r^{safety} negative feedback on adverse drug reactions (ADRs), the intensity of which is correlated with the severity of ADRs, and potential risks are predicted using contraindications and interaction relationships in the knowledge graph. The complexity and cost of compliance items $r^{compliance}$ minor adjustment plans.

Strategy learning adopts the Actor Critic architecture, where the Actor network receives the state st 'and outputs the probability distribution of actions. Critic network evaluates state value and provides low variance advantage estimation to optimize policy gradient updates. The intelligent agent interacts in a simulated environment constructed from historical electronic medical records, using an experience replay buffer to store transfer samples (s_t, a_t, r_t, s_{t+1}) for batch training. Integrating knowledge graph logic into environmental state transition ensures that decisions comply with medical constraints.

During the deployment phase, a fully trained intelligent agent generates the most probable medication action at based on real-time patient status st'. This module endows the system with the ability to dynamically track patient status evolution and optimize long-term benefits, and is the core driver for KG-DRL to achieve personalized and accurate recommendations.

4. Experiment and Results

Dataset and setup: Experimental integration of multi-source medical knowledge graph (Dr ugBank, PharmGKB, ICD-10), covering 15K drugs, 8K disease entities, and over 1.2M tripl ets. The patient medication records were sourced from the MIMIC-III v1.4 clinical database that had undergone desensitization treatment. A diagnosis and treatment sequence of 50000 patients was constructed, and the training/validation/testing sets were divided into 7:1.5:1.5. The baseline comparison covers traditional methods (POP, KNN), collaborative filtering (B PR-MF), deep models (FM, DeepFM), knowledge graph models (KGCN, RippleNet), and D RL without knowledge graph (DRL NoKG). Evaluation indicators include recommendation a ccuracy（ Accuracy@5 ， Recall@5 ， F1@5 ， MRR）、Novelty（Novelty@5）And core med ical indicators - Avoidable ADR Rate and ΔEfficiency.

Table 1. Key Recommendation Performance Comparison

Model	Accuracy@5	Recall@5	F1@5	MRR	Novelty@5
POP	0.1821	0.2103	0.1952	0.1247	0.0512
KNN	0.2536	0.2874	0.2693	0.1983	0.1038
BPR-MF	0.3017	0.3421	0.3205	0.2569	0.1527
FM	0.3258	0.3689	0.3456	0.2814	0.1689
DeepFM	0.3482	0.3925	0.3689	0.3057	0.1853
KGCN	0.3715	0.4180	0.3932	0.3316	0.1721
RippleNet	0.3628	0.4103	0.3848	0.3240	0.1654
DRL	0.3893	0.4372	0.4118	0.3498	0.1785
KG-DRL	0.4287	0.4816	0.4536	0.4021	0.1796

Overall, KG-DRL outperforms all baseline models significantly in all core recommendation metrics. This demonstrates the effectiveness of combining knowledge graph semantic information with reinforcement learning sequence decision-making ability. Compared to DRL without KG, the improvement of KG-DRL is particularly significant, highlighting the key role of medical knowledge graph embedding in accurately understanding patient status and drug characteristics. DeepFM and KGCN models also utilize feature interaction or graph information, but lack the ability to model dynamic decision-making processes and long-term benefits. The novelty of

KG-DRL is slightly lower than DeepFM, but significantly higher than traditional methods such as POP and KNN, and comparable to KGCN, RippleNet, and DRL (No KG). This indicates that KG-DRL, while pursuing precise recommendations, is not overly conservative and can explore reasonable new regimens that are different from the patient's previous medication. The high novelty of DeepFM may stem from its stronger data fitting ability, but it may also bring higher risks.

5. Conclusion

This study proposes a knowledge graph enhanced deep reinforcement learning framework (KG-DRL) to address the two core bottlenecks of insufficient knowledge fragmentation integration and difficulty in tracking user dynamic needs in medical recommendation systems. By constructing a high-order medical knowledge graph that integrates multiple types of entities such as drugs, diseases, and patients, and innovatively using a meta path guided Graph Attention Network (GAT) to model deep semantic associations, the system breaks through the limitations of traditional methods in expressing complex medical logic. Further design a sequence decision-making mechanism based on DRL, embed knowledge graph dynamically into patient state representation and reward function, achieve long-term efficacy safety optimization of personalized medication plans, and provide a knowledge driven intelligent decision-making paradigm for the medical industry.

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