DIALMED: A Dataset for Dialogue-based Medication Recommendation

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Abstract

Medication recommendation is a crucial task for intelligent healthcare systems. ous studies mainly recommend medications with electronic health records (EHRs). However, some details of interactions between doctors and patients may be ignored or omitted in EHRs, which are essential for automatic medication recommendation. Therefore, we make the first attempt to recommend medications with the conversations between doctors and patients. In this work, we construct DIALMED, the first high-quality dataset for medical dialogue-based medication recommendation task. It contains 11,996 medical dialogues related to 16 common diseases from 3 departments and 70 corresponding common medications. Furthermore, we propose a Dialogue structure and Disease knowledge aware Network (DDN), where a QA Dialogue Graph mechanism is designed to model the dialogue structure and the knowledge graph is used to introduce external disease knowledge. The extensive experimental results demonstrate that the proposed method is a promising solution to recommend medications with medical dialogues. The dataset and code are available at https://github.com/ f-window/DialMed.

1 Introduction

The outbreak of COVID-19 has challenged the healthcare systems and led to millions of patients facing delays in diagnosis and treatment. As an essential complement to the traditional face-to-face medicine, telemedicine relieved the therapeutic stress caused by the diversion of medical resources. According to the report of WeDoctor¹, an online health consultation platform in China, about 1.2 million patients conducted online medical consultations during the COVID-19 Pandemic.

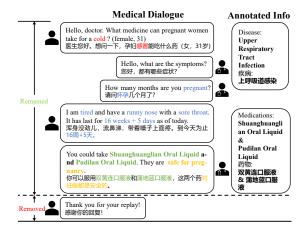


Figure 1: A typical medication consultation dialogue. Here, the disease is *Upper Respiratory Tract Infection*, and the medication is *Shuanghuanglian Oral Liquid* and *Pudilan Oral Liquid*.

Telemedicine can increase the availability of medical treatment, reduce healthcare costs, and improve the quality of care. Consequently, it has attracted increasing attention due to its vast application potential.

Our study found that around 31% of online consultations are about what medications the patients should take based on their current conditions². Figure 1 demonstrates a typical medication consultation dialogue. The patient reported the health issues initially, with some personal information, such as gender and age. Then the doctor asked for further information (*e.g.*, symptoms and disease history) about the patient. Finally, the doctor provided medication advice based on the gathered information and clinical experience.

Existing studies on medication recommendation are primarily based on EHRs (Zhang et al., 2017; Shang et al., 2019b; An et al., 2021), accumulatively collected according to a diagnostic procedure in clinics. However, the doctors will omit some details of interactions with patients in EHRs,

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¹https://www.guahao.com/

²Refer to Appendix D.1 for details of statistic.

which are essential for the automatic medication recommendation. Compared to EHRs, medical dialogues retain original interactions between doctors and patients, containing more rich information. To this end, medical dialogue-based medication recommendation is a promising and challenging task.

Therefore, in this work, we study the new task, namely dialogue-based medication recommendation. Due to the lack of available datasets, we firstly construct a high-quality online medical dialogues dataset (DIALMED) for this task. It contains 11,996 consultation dialogues, 16 diseases from 3 different departments, and 70 related common medications.

Then, to further advance the research of this task, we propose a Dialogue structure and Disease knowledge aware Network (DDN). In DDN, for the input dialogue, we first utilize a pre-trained language model to extract the semantic information of each utterance. A mechanism named QA Dialogue Graph is designed to understand the questions&answers implied in utterances, and then we apply graph attention network on this QA graph to get the dialogue embedding. Meanwhile, for the input disease, we use its identity to query the entity in a knowledge graph CMeKG³, and input the dialogue embedding to a graph attention network to get contextual disease embedding. The two embeddings are fused to make the medication prediction. Moreover, we conduct extensive experiments to show that the proposed method can effectively recommend medications with medical dialogues.

Our contributions can be summarized as follows:

- We construct the first high-quality humanannotated dialogue dataset for dialogue-based medication recommendation task.
- We propose a novel medication recommendation framework which models dialogue structure with QA Dialogue Graph and introduces external disease knowledge.
- We conduct extensive experiments to demonstrate DDN can extract the essential information to make medication recommendation effectively.

2 Related Work

Medication Recommendation. Existing medication recommendations are mainly based on

It could be categorized into instancebased and longitudinal-based recommendation methods (Shang et al., 2019b). Instance-based methods are based on the current health conditions extracted from recent visit (Zhang et al., 2017; Wang et al., 2019a). For example, (Zhang et al., 2017) proposed a multi-instance multi-label learning framework to predict medication combination based on patient's current diagnoses. Longitudinalbased methods leverage the temporal dependencies among clinical events (Choi et al., 2016; Le et al., 2018; Shang et al., 2019b,a; Wang, 2020; He et al., 2020; Wang et al., 2021; Yang et al., 2021). Among them, (Shang et al., 2019a) combined the power of graph neural networks and BERT for medication recommendation. (Yang et al., 2021) proposed a drug-drug interactions (DDI)-controllable drug recommendation model to leverage drugs' molecule structures and model DDIs explicitly.

Unlike the work mentioned above, dialogue-based medication recommendation task is more challenging in practice due to the noisy and sparse data. Because of the privacy issue, it is difficult to get historical dialogues of a patient on online consultation platforms. So we perform the medication recommendation solely based on the current medical dialogues.

Graph Neural Networks. Graph neural networks have attracted a lot of attention for processing data with graph structures in various domains (Zhou et al., 2020). For example, (Kipf and Welling, 2017) proposed the graph convolutional networks (GCN). With integration of attention mechanisms, graph attention networks (GAT) (Veličković et al., 2018) has become one of the most popular methods in graph neural networks.

Recently, some works have applied GAT to the dialogue modeling. (Chen et al., 2020) used Graph attention and recurrent GAT to fully encode dialogue utterances, schema graphs, and previous dialogue states for dialogue state tracking. (Qin et al., 2020) proposed a co-interactive GAT layer to simultaneously solve both dialog act recognition and sentiment classification task. In this work, we utilize GAT to model the intra- and inter-speaker correlations to propagate semantic on the QA Dialogue Graph and extend the GAT on knowledge graph to introduce external knowledge.

³http://cmekg.pcl.ac.cn/

3 Corpus Description

In this section, we introduce the construction details and statistics of DIALMED, and its comparison with other studies.

3.1 Construction Details

Our dataset is collected from Chunyu-Doctor⁴, which is a popular Chinese medical consultation website for doctors and patients. The conversations between doctors and patients contain rich but complex information, mainly related to the patients' current conditions. The diagnosed diseases and symptoms both are indispensable for accurate medication recommendation. Considering the complexity of the symptoms, we decide to utilize information from explicit disease and implicit symptoms in this paper. So we annotate the diagnosed diseases and recommended medications (replaced with a mask token to keep the original dialogue structure). For the example in Figure 1, we annotate the disease Upper Respiratory Tract Infection, and replace the medications Shuanghuanglian Oral Liquid and Pudilan Oral Liquid with special token [MASK]. Moreover, the future utterances after the point of recommendation are removed to make DIALMED more realistic, as the decision of doctors should not be influenced by future contexts.

The procedure of annotation consists of two parts, labeling and normalization of medications and diseases. First, we select 16 common diseases and the corresponding common medications from 3 departments (i.e., respiratory, gastroenterology, and dermatology) with the guidance of a doctor. These diseases have abundant medication consultations online. Then three annotators with relevant medical backgrounds are involved. Each dialogue is annotated by two annotators and will be further judged by another one if there is any inconsistency. The annotation consistency, i.e., the Cohen's kappa coefficient (Fleiss and Cohen, 1973) of the labelled dialogues is 88.4%. For the quality of dataset, conversations containing unsuitable medications for patients would be discarded.

Secondly, we normalize the medications since there are many generic names, trade names, or colloquial expressions for the same drug in dialogues. Specifically, different brands of the same drug are grouped into one cluster and normalized as a common name from DXY Drugs Database⁵. For

example, Omeprazole enteric-coated tablet and Omeprazole tablet are normalized to Omeprazole. Similarly, we normalize the different names of diseases into ICD-10 standard names. The dialogues, hard to give diagnosed diseases or given diseases out of our scope, would be marked as a special placeholder, None or Others.

3.2 Dataset Statistics

Top of Table 2 summarizes the statistics of DIALMED. The scenario of dialogues in the dataset is similar to outpatient procedure, so the number of medicines per dialogue is relatively small. Then, the frequency of medications and diseases are shown in Figure 2(a) and Figure 2(b) respectively. The distributions of quantity demonstrate that DIALMED aligns with the real-world case.

Compared to the other medical dialogue datasets in Table 1, our dataset has three advantages: (1) DIALMED has the largest volume among the manual annotation datasets, as unlabeled datasets are mainly constructed for the task of dialogue generation. (2) Though the future contexts after recommendation are removed, the average number of dialogue turns in DIALMED still remains high compared to other datasets. It is mainly benefited from our evaluation for inclusion of short dialogues in DIALMED during the labeling process. (3) We carefully choose the fields suitable for medication recommendation and avoid coarsely expanding the scope of medical domains, which makes DIALMED have a higher quality.

The panoramas of medications & diseases' frequency could be found in Appendix D.2.

3.3 The comparison with other studies

To our best knowledge, DIALMED is the first dataset for the medication recommendation based on medical dialogues. It has the following differences with the existing work.

Dataset Medical dialogue has attracted increasing attention in recent years. Although there are medication mentions in many medical dialogue datasets, the distributions are fragmentary and the authors do not categorize and normalize these drug mentions which would lead to label explosion. For instance, medication mentions, **Omeprazole entericcoated tablet**, **Omeprazole tablet** and **Omeprazole**, which may occur in dialogues would be three classes without normalization. In fact, they are essentially equivalent in the eyes of doctors. By

⁴https://www.chunyuyisheng.com/

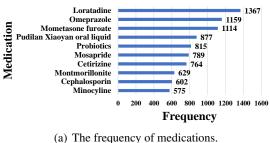
⁵http://drugs.dxy.cn/

Dataset	#Task	#Domain	#Disease	#Dialogue	#Avg. Turn	#Annotation
MZ(Wei et al., 2018)	Diagnosis	Pediatrics	4	710	-	Man.
DX(Xu et al., 2019)	Diagnosis	Pediatrics	5	527	5.34	Man.
CMDD(Lin et al., 2019)	Diagnosis	Pediatrics	4	2,067	42.09	Man.
SAT(Du et al., 2019)	Extraction	14		2,950	-	Man.
MIE(Zhang et al., 2020)	Extraction	Cardiology	6	1,120	16.19	Man.
MSL(Shi et al., 2020)	Extraction	Pediatrics	5	2,652	-	Man.
MedDG(Liu et al., 2020)	Extraction	Gastroenterology	12	17,864	21.60	Man.& Semi-Auto.
COVID-EN(Yang et al., 2020)	Generation	COVID-19	1	603	8.7	None
COVID-CN(Yang et al., 2020)	Generation	COVID-19	1	1088	2.0	None
MedDialog-EN(Zeng et al., 2020)	Generation	51	96	257,332	2	None
MedDialog-CN(Zeng et al., 2020)	Generation	29	172	3,407,494	3.3	None
Chunyu(Lin et al., 2021)	Generation	-	15	12,842	24.7	Rule
KaMed(Li et al., 2021)	Generation	100	-	63,754	11.62	None
ReMeDi(Yan et al., 2022)	Diag.&Ext.&Gene.	30	491	1,557	16.34	Man.
DIALMED(ours)	Medication	R&G&D	16	11,996	10.94	Man.

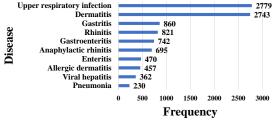
Table 1: Comparison between our dataset and other related medical dialogue datasets. Extraction, Generation and Medication mean information extraction, dialogue generation and medication recommendation separately. R&G&D, Man. and Semi-Auto are abbreviations of Respiratory&Gastroenterology&Dermatology, Manual and Semi-Automated respectively.

	#Dial.	#Dise.	#Med.	Avg.M	Avg.T	Max.T	Avg.U	Max.U
Resp.	4,859	4	45	2.06	10.76	52	18.18	374
Gastro.	3,818	9	39	1.88	13.05	58	16.70	463
Derma.	3,319	3	27	1.62	8.77	44	18.82	453
Total	11,996	16	70	1.88	10.94	58	17.76	463
Train.	9,605	16	70	1.88	10.95	58	17.74	463
Dev.	1,192	16	70	1.89	11.25	49	17.45	298
Test.	1,199	16	70	1.89	10.58	42	18.27	293

Table 2: Data statistics of DIALMED. M, T, and U represent medicine, dialogue turns, and utterance.



spiratory infection



(b) The frequency of diseases.

Figure 2: The frequencies of medications and diseases. Top 10 are exhibited for the constraint of space.

contrast, we reduce the complexity caused by the doctors' preferences for different brands through categorization and normalization. DIALMED is developed for drug recommendation.

Task Drug recommendation is a sub-task of medical diagnosis. According to patients' questions, the objectives of current diagnosis systems are to generate the optimal clinical responses which may be intended as one of greeting, inquiry or diagnosis. Even if there contains drug mentions in responses, it is just one of the system's options. Drug recommendation is a key task and requires specialized dataset. DIALMED goes a step forward.

Scenario There are remarkable distinctions between DIALMED and MIMIC-III (Johnson et al., 2016), an EHR database which is relied on in current medication recommendation study. The scenario of the former is outpatient procedure while the data from the latter is generated from Intensive Care Units (ICU). In MIMIC-III, for example, the number of medications is 145, the average number of medications in each visit is 8.80, and the average number of diagnosis in each visit is 10.51. In contrast, the labels in medical dialogues are relatively sparse, leading to a more challenging task.

4 Our Approach

In this section, we first introduce the dialoguebased medication recommendation task, and then describe the proposed DDN in detail.

4.1 Problem Formulation

In the online medical dialogue setting, each dialogue consists of a sequence of utterances from the patient and the doctor. Formally, each dialogue can be represented as $\mathcal{D}_n = \{u_1, u_2, ..., u_{|\mathcal{D}_n|}\},\$ where $n \in \{1, 2, ..., N\}$, N denotes the total number of dialogues in the dataset, and $|\mathcal{D}_n|$ represents the number of utterances in a dialogue \mathcal{D}_n . Each utterance can be represented as $u_i =$ $\{w_i^1,...,w_i^j,...,w_i^{|u_i|}\}$, where w_i^j is the j-th word in u_i and $|u_i|$ denotes the number of words in u_i . We collect all the diseases and medications mentioned in the dataset to construct a disease corpus S and medication corpus M. To avoid notation clutter, we hereinafter remove the subscript n as we only consider a single dialogue instance. Formally, given the consultation dialogue \mathcal{D} and the diagnosed disease d as inputs, dialogue-based medication recommendation aims to recommend potential treatment medications y in \mathcal{M} , where $\mathbf{y} \in \{0,1\}^{|\mathcal{M}|}.$

4.2 Model Overview

The proposed end-to-end framework is presented in Figure 3, consisting of two parts: (1) Dialogue Encoder, encoding the medical dialogues between patient and doctor by comprehensively capturing the semantic information and dialogue structure. (2) Disease Encoder, incorporating external medical knowledge based on the disease information from the dialogue and knowledge graph.

4.3 Dialogue Encoder

Dialogues contain two types of important information: (1) the rich semantic information, (2) strong structural correlations between utterances.

Utterance Encoding Pre-trained language models (e.g., RoBERTa) are utilized to capture the semantic information in utterances. First, special tokens [CLS] (capturing utterance representation) and [SEP] (separating different utterances) are inserted at the beginning and end of each utterance token sequence u_i . Then the position embedding of each token in a utterance is calculated. In addition, two types of speaker embeddings (i.e., Doctor and Patient) are proposed to make model aware of the speaker role of the utterance. The model takes the sum of three embeddings as input and outputs the representation of [CLS] as the utterance embedding \mathbf{h} . So a dialogue \mathcal{D} can be represented as $\mathbf{h}_D = \{\mathbf{h}_1, \mathbf{h}_2, ..., \mathbf{h}_{|\mathcal{D}|}\}$.

QA Dialogue Graph In medical conversations, the interactions between doctors and patients tend to be in the form of questions and answers. For example, in Figure 3, the doctor asked two questions in u_2 and u_3 , and the patient gave the answers in u_4 . So it's important to capture the structure of QA pairs in conversation in order to understand the whole medical dialogue. We propose a new method to model the dialogue based on the observation that there is a high possibility of question-and-answer relations between adjacent utterances.

Specifically, we design a mechanism named QA Dialogue Graph, where each utterance is represented as a node in graph, and consecutive utterances spoken by the same speaker is represented as a block, e.g., u_2 and u_3 constitute a block with two nodes, and u_4 is another block with one node. Then the constructions of edges between nodes can be defined as follows:

- Within a block, each node connects with all other nodes in the block. This represents the intra-speaker correlation and ensures the information from the same speaker propagates among utterances within a local context.
- For two adjacent blocks, each node in a block connects with all nodes in the other block.
 This represents the inter-speaker correlation and ensures the information flow between doctors and patients within consecutive contexts.

An example of the adjacency matrix of the dialogue is shown in Figure 3. In general, when compared to previous works on dialogue modeling, QA Dialogue Graph has two advantages. Firstly, the construction of graphs does not require additional supervised information (Joshi et al., 2021; Feng et al., 2021). Secondly, our method comprehensively captures the structural and semantic information of QA pairs, which is key to understanding conversations (Qin et al., 2020; Shen et al., 2021b).

Dialogue Encoding GAT is employed to automatically aggregate semantic and structure features on QA Dialogue Graph. In particular, the *l*-th layer representation of a vertex can be computed as:

$$\mathbf{h}_{i}^{(l)} = \sigma\left(\sum_{j \in \mathcal{N}_{i}} \alpha_{ij} W_{h} \mathbf{h}_{j}^{(l-1)}\right) \tag{1}$$

where \mathcal{N}_i is the first-order neighbors of vertex i, $W_h \in \mathbb{R}^{d_l \times d_{l-1}}$ is a trainable weight matrix, and σ is a nonlinear activation function. The weight

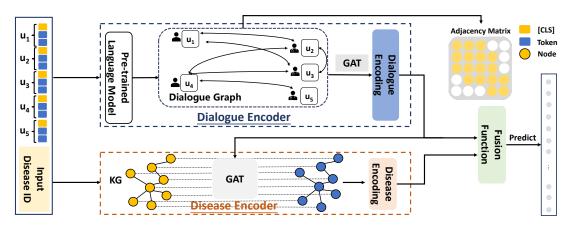


Figure 3: The framework of the proposed DDN for dialogue-based medication recommendation.

 α_{ij} which determines the relatedness between two vertices can be calculated following (Veličković et al., 2018):

$$\alpha_{ij} = \frac{\exp\left(\sigma(\mathbf{a}^T W_h[\mathbf{h}_i || \mathbf{h}_j])\right)}{\sum_{k \in \mathcal{N}_i} \exp\left(\sigma(\mathbf{a}^T W_h[\mathbf{h}_i || \mathbf{h}_k])\right)}$$
(2)

where $\mathbf{a} \in \mathbb{R}^{2d_l}$ is a trainable weight matrix, and σ is the LeakyReLU activation function. Finally, we apply the attention pooling on nodes embedding to obtain the dialogue representation $\mathbf{h}_{\mathcal{D}}$, where \mathbf{W}_a is a learnable parameter and $\mathbf{h}^{(l)}$ is the representation of utterances after l^{th} layer.

$$\widehat{\alpha} = softmax(\mathbf{W}_a \mathbf{h}^{(l)}) \tag{3}$$

$$\mathbf{h}_{\mathcal{D}} = \sum_{i} \widehat{\alpha}_{i} \mathbf{h}_{i}^{(l)} \tag{4}$$

4.4 Disease Encoder

Disease knowledge is crucial for delivering accurate medication recommendation. In this paper, we incorporate knowledge from CMeKG, a high-quality Chinese medical knowledge graph. TransR (Wang et al., 2019b) is utilized to get the initial entities embedding. Given a disease d, we first identify the corresponding entity in CMeKG, and then a KG subset with K hops starting from the disease entity is sampled randomly, finally the GAT network is used to get the disease embedding under the dialogue context.

Here, we fuse the entity, relation and dialogue information to get the attention scores:

$$\beta_{ij} = \frac{\exp\left(\sigma(\mathbf{a}^{T}[W[\mathbf{h}_{i}, \mathbf{h}_{j}] || W_{r}\mathbf{r}_{\varphi} || W_{D}\mathbf{h}_{\mathcal{D}}])\right)}{\sum_{j \in \mathcal{N}_{i}} \exp\left(\sigma(\mathbf{a}^{T}[W[\mathbf{h}_{i}, \mathbf{h}_{j}] || W_{r}\mathbf{r}_{\varphi} || W_{D}\mathbf{h}_{\mathcal{D}}])\right)}$$
(5

where σ is the LeakyReLU function, \mathbf{h}_i , \mathbf{h}_j and \mathbf{r}_{φ} are the embeddings of node i, j and their relation

separately. And W, W_r , and W_D are learnable weights to transform node, relation and dialogue embeddings, respectively. Then the l-th layer of disease embedding can be obtained as follows:

$$\mathbf{s}_{i}^{(l)} = \sigma\left(\sum_{j \in \mathcal{N}_{i}} \beta_{ij} W_{k} \mathbf{h}_{j}^{(l-1)}\right) \tag{6}$$

The contextual embedding of last layer is the disease d's representation, denoted by \mathbf{s}_d .

For dialogues with None or Others placeholder rather than a disease label, a learnable vector $\hat{\mathbf{s}}_d$ would be assigned to \mathbf{s}_d .

4.5 Model Inference and Optimization

The dialogue h_D and disease s_d are fused by the fusion function to make prediction. In this work, we concatenate them and then fed it into decoder to make the medication prediction as follows:

$$\mathbf{y} = \sigma(W_o[\mathbf{h}_D; \mathbf{s}_d] + \mathbf{b}_o) \tag{7}$$

where $W_o \in \mathbb{R}^{|\mathcal{M}| \times 2d}$ and $\mathbf{b}_o \in \mathbb{R}^{|\mathcal{M}|}$ are trainable weight matrices for the decoder, σ is the sigmoid activation function. Here, we reserve all the candidates whose probability is higher than the threshold of 0.5 as the recommended treatment medication combination.

Since medication combination recommendation is treated as a multi-label classification task (Shang et al., 2019b; Yang et al., 2021), we utilize the binary cross-entropy loss as the objective function, which can be formulated as:

$$\mathcal{L} = -\sum_{i=1}^{|\mathcal{D}|} \sum_{j=1}^{|\mathcal{M}|} (y_j^{(i)} \log \widehat{y}_j^{(i)} + (1 - y_j^{(i)}) \log(1 - \widehat{y}_j^{(i)}))$$
(8)

where $|\mathcal{D}|$ is the number of dialogues in the training set, $|\mathcal{M}|$ is the number of medications. $y_j^{(i)}$ is the ground truth label which equals 1 if medication

j is prescribed by the doctor in dialogue i, and 0 otherwise. $\widehat{y}_{j}^{(i)}$ is the predicted probability of recommending medication j.

5 Experiments

5.1 Experimental Setup

Dataset In our experiments, we divide the data into train/development/test dialogue sets as shown in Table 2. The average number of medications in each dialogue is approximately the same, as well as the the average length of utterances and dialogues, meaning the distribution of the data is relatively consistent among three sets.

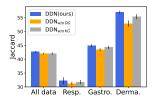
Implementation Details The pretained model we use is Chinese RoBERTa-base model. The learning rate and the batch size are set as 2×10^{-5} and 8, respectively. Adam optimizer is utilized to optimize the model. All methods are implemented and trained using Pytorch on GeForce RTX 3090 GPUs. The results are the mean of five trainings.

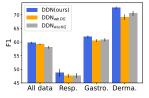
Baselines Since there is no standard baselines for this task, we implement several methods of related tasks, including statistics-based (i.e., TF-IDF (Salton and Buckley, 1988)), RNN-based (i.e., LSTM-flat, LSTM-hier, RETAIN (Choi et al., 2016) and DAG-ERC (Shen et al., **2021b**)), and transformer-based methods (i.e., **Hi**-**TANet** (Luo et al., 2020), **LSAN** (Ye et al., 2020)) and DialogXL (Shen et al., 2021a). The RETAIN, HiTANet and LSAN are strong baselines for EHRbased medication recommendation or risk prediction. DAG-ERC and DialogXL are the SOTA methods at Emotion Recognition in Conversation (ERC). Among them, LSTM-hier takes the dialogue structure into consideration, and LSAN and DialogXL are modified to incorporate disease knowledge. Refer to Appendix B.1 for more details.

Evaluation Metrics We adopt two commonly used metrics, namely **Jaccard** and **F1** scores, to evaluate the model performance.

5.2 Main Results

Table 3 shows performances of all methods under the metric of Jaccard and F1 on four datasets. The results clearly indicate that DDN has achieved the best performances among all baselines. Particularly, DDN improves 6.35%, 5.14%, 3.95%, and 8.31% compared with the second best method (i.e., **DialogXL**) at Jaccard, respectively. Further,





(a) Jaccard on four datasets

(b) F1 on four datasets

Figure 4: Performance comparison of DDN and its variants.

RETAIN and LSTM-hier outperform LSTM-flat, demonstrating the dialogue structure is important for the dialogue understanding. And LSAN, DialogXL outperforms HiTANet, indicating that disease knowledge is also essential for the dialogue modeling. Our well-designed model DDN considers both of the above and achieves the best performance. In addition, it is worth noting that the performance varies over three departments, which may attribute to the considerable difference of medication and disease frequencies between different departments.

5.3 Ablation Study

Figure 4 summarizes the contributions of QA Dialogue Graph and disease knowledge of our model. We notice that by removing the QA Dialogue Graph, the variant $\mathrm{DDN}_{w/o\ DG}$ shows considerable performance decrease at both Jaccard and F1 compared with DDN, especially on three departments datasets. It demonstrates that dialogue graph structure is important for the medical information extraction in dialogue-based medication recommendation task. Similarly, by removing the Knowledge Graph module, $\mathrm{DDN}_{w/o\ KG}$ also shows similar performance decrease trends, indicating that disease knowledge can improve the medication recommendation performance. This is reasonable and accords with the actual medication consultation situations.

5.4 Task Feasibility Analysis

To prove the feasibility of dialogue-based medication recommendation, we provide incomplete discourses to DDN during the inference process to explore whether the dialogue can provide necessary medical information. Figure 5 shows the model performances under different portions of discourses. We can see that with the increasing of dialogue discourse percentage, the performance gets better, especially within the first 20% and the last 20%.

		All	Data	Respi	ratory	Gastroei	iterology	Derma	itology
Type of Model	Model	Jaccard	F1	Jaccard	F1	Jaccard	F1	Jaccard	F1
Statistics	TF-IDF(Salton and Buckley, 1988)	$21.25{\pm}0.41$	35.05 ± 0.56	16.06 ± 0.44	27.68 ± 0.66	$23.85{\pm}0.40$	$38.52{\pm}0.52$	$28.84{\pm}0.14$	44.77±0.17
	LSTM-flat	27.50±1.09	42.54±1.22	18.07±0.44	30.18±0.64	31.31±1.33	47.18±1.59	32.69±1.71	48.55±1.18
RNN-Based	LSTM-hier	$30.20{\pm}0.47$	$46.39 {\pm} 0.56$	$22.86 {\pm} 0.42$	37.21 ± 0.56	$32.90{\pm}0.93$	$49.51\!\pm\!1.05$	36.00 ± 0.50	$52.94{\pm}0.54$
	RETAIN(Choi et al., 2016)	$31.16{\pm}0.82$	$42.16{\pm}0.99$	$21.13 {\pm} 0.64$	$30.49{\pm}0.96$	36.70 ± 0.86	$48.54 {\pm} 0.73$	$43.19{\pm}1.06$	$54.14{\pm}1.20$
	DAG-ERC(Shen et al., 2021b)	$29.08 {\pm} 0.56$	$44.05\!\pm\!0.70$	$23.74 {\pm} 0.76$	$35.71 \!\pm\! 1.02$	$36.16{\pm}0.46$	$53.80 {\pm} 0.52$	$31.18{\pm}1.05$	$47.52 {\pm} 1.23$
	HiTANet(Luo et al., 2020)	30.75±0.69	44.57±0.83	22.01±1.04	33.62±1.44	33.95±1.26	48.39±1.26	39.17±1.93	53.41±2.21
Transformer	LSAN(Ye et al., 2020)	$34.33{\pm}0.58$	$46.14 {\pm} 0.45$	$26.11\!\pm\!1.06$	$38.89{\pm}1.01$	$39.28{\pm}0.22$	52.49 ± 0.62	$50.29 {\pm} 1.24$	57.90 ± 1.09
	DialogXL(Shen et al., 2021a)	$36.27{\pm}0.34$	53.23 ± 0.40	$27.12 {\pm} 0.24$	$42.67 {\pm} 0.36$	$40.91 {\pm} 0.14$	$58.06 {\pm} 0.15$	$48.68 {\pm} 0.81$	$65.48 \!\pm\! 0.66$
	DDN(Ours)	$42.62 {\pm} 0.35$	$59.77 \!\pm\! 0.34$	$32.26\!\pm\!1.25$	$48.77 {\pm} 1.43$	$44.86 {\pm} 0.54$	$61.93 \!\pm\! 0.52$	$56.99 {\pm} 0.53$	$72.60 \!\pm\! 0.43$

Table 3: Performance (%) comparison of DDN with baseline methods over the overall and three departments datasets. The best result in each column is highlighted in boldface. The performance gain of our method over all baselines is statistically significant with p < 0.05 under t-test.

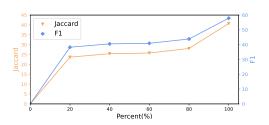


Figure 5: Average Jaccard scores on different percents(%) of dialogue discourse. In this setting, we choose dialogues with more than four turns in test set.

This may be because that the first and last parts of dialogue contain much patient complaints and symptoms that are closely related to the medications. The results demonstrate that recommending medication based on medical dialogues is feasible.

5.5 Error Analysis

Although we have elaborately designed a model for the task, the results are not so well satisfactory. So we make detailed analysis of the error cases in the test set. Table 4 summarizes the statistics of our defined five type of errors. We can see that (1) 86.38% of the cases (#3, #4, #5) predict wrong medications, which is mainly caused by DDN failing to distinguish the medications with similar effect. (2) 7.20% of the cases predict none labels, which can be attributed to that these dialogues provide a little disease-related information.

No.	Type of error	# Cases
#1	$P \subseteq \emptyset$	65(7.20%)
#2	$P \subset T \& P \not\subseteq \emptyset$	58(6.42%)
#3	$T \subset P$	182(20.16%)
#4	$T \not\subseteq P \& P \not\subseteq T \& P \cap T \not\subseteq \emptyset$	299(33.11%)
#5	$T \not\subseteq P \& P \not\subseteq T \& P \cap T \subseteq \emptyset$	299(33.11%)
Total	-	903

Table 4: The statistics of errors on test set. P and T are the predicted and golden label set, respectively.

Sample	Medications		
Disease: Duodenitis P: Hello, doctor. In March this year, I had a	TF-IDF	Omeprazole Digestive enzymes 2 Missed	
duodenal ulcer, bleeding, and was hospita lized. Stomach rises a bit uncomfortable a	LSTM-flat	Omeprazole 2 Missed	
nd bloating in the night a week recently. I s it recrudescent?	LSTM-hier	Omeprazole Mosapride Digestive enzymes	
D : Duodenal ulcers are indeed prone to recurrence or inflammation. P : Can you prescribe some medicine for me?	RETAIN	1 Missed Mosapride 2 Missed	
I don't have time to go to the hospital right now.	DAG-ERC	Omeprazole 2 Missed	
D : Besides what you said, do you have any oth er complaints? Like acid reflux, heartburn.	HiTANet	Mosapride 2 Missed	
P: No. What does heartburn mean? I don't ha ve this feeling at ordinary times. At presen	LSAN	Omeprazole 2 Missed	
t, I wake up uncomfortably in some nights.	DialogXL	Omeprazole 2 Missed	
P: Almost no symptoms during the day. D: I suggest you take [MASK], [MASK], [MASK].	DDN(Ours)	Omeprazole Mosapride Glutamine	

Figure 6: The sample is extracted from the DIALMED test set. Golden labels of this case are Omeprazole, Mosapride and Glutamine. The "Missed" means the medication is in golden labels but not be predicted, and the underlined drugs in red represent the predicted medications that are not in ground truth.

5.6 Case Study

We further provide a case study to illustrate the superiority of DDN. Figure 6 shows the medical dialogue and the medications recommended by all baselines and our method. The baselines either miss some medications, e.g., LSTM-flat, RETAIN, HiTANet, LSAN, or give the wrong drugs, e.g., TF-IDF, LSTM-hier. DDN takes full account of Duodenitis-related information from the dialogue (e.g., the symptoms in chief complaint and past medical history) and the external knowledge graph. It recommends Omeprazole (inhibiting gastric acid secretion) and Mosapride (promoting gastric dynamics), as well as Glutamine which is omitted by all baselines.

6 Conclusions

In this paper, we studied a new task, namely dialogue-based medication recommendation. First, we presented the first high-quality medical dialogue dataset DIALMED for this task. And then we implemented several baselines, as well as designed a dialogue structure and external disease knowledge aware model. Experimental results show that medication recommendation quality can be enhanced with the help of dialogue structure and external disease knowledge.

Ethical considerations

Data in DIALMED is publicly collected from Chunyuyisheng, and personal information (e.g., usernames) is preprocessed. The annotating process is as described in Section 3. Furthermore, to ensure the quality of dataset, we paid the annotators 1 yuan (\$0.16 USD) per label. The applications of machine learning in medical treatment would inevitably raise ethical issues. But the research on AI medicine should not be stopped by this, since the purpose of such research is how to make machines better serve human beings. We have seen many advanced achievements (Lin et al., 2021; Li et al., 2021; Zhang et al., 2020; Liu et al., 2020; Lin et al., 2019; Xu et al., 2019; Wei et al., 2018) in this field. For this study, the ethical issue is that there may cause bad cases in practical application. However, individual errors could be reduced by making doctors responsible for decisions while machines are used as assistants.

Acknowledgements

This research was partially supported by National Key R&D Program of China under grant No. 2018AAA0102102, National Natural Science Foundation of China under grants No. 62176231 and 62106218, Zhejiang public welfare technology research project under grant No. LGF20F020013. The authors would thank Ruochen Yan for her help in data processing.

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A Corpus

A.1 Details of corpus construction

First of all, diseases and related medications were identified in a dialogue. Secondly, we selected and annotated those dialogues containing drugs in our medication list. To speed up tagging process, we built an annotation tool based on this task. For each raw medical dialogue, the annotators need to annotate the disease of patients and medications recommended by doctors. We believe that the context after the doctor recommending the drug is not meaningful for drug inference. Due to the emergence of new medications in the labeling process and existence of ambiguity on recommendation, two additional annotation processes were carried out. Next we will focus on the processing of diseases and medications.

Disease Processing. With the guidance of a doctor, we select 16 diseases from 3 departments (i.e., respiratory, gastroenterology and dermatology) with following reasons: (1) they are common diseases and research on them have more practical value. (2) they could be consulted online and there are abundant medication consultations. As described by Section Corpus Description, we normalize the diseases to improve the quality of DIALMED, e.g., chronic gastritis and acute gastritis are mapped to gastritis. The dialogues without explicit disease information or diseases in our scope were marked as None or Others. We mark one disease according to the chief complaint of patients who have more than one disease, because patients have only one complaint in most diagnostic scenarios.

Medication Processing. As for medications, the ones we choose are commonly prescribed by doctors. Considering the differences between traditional Chinese medicines and Western medicine, both are included to achieve complementary advantages. Since there are many generic names, trade names and colloquial expressions for the same drug in conversations, it is significant to normalize the drug to a single label. For example, Omeprazole enteric-coated tablet and Omeprazole enteric-coated capsule could be mapped to Omeprazole. For compound medicines, we combine drugs that have the same ingredients into one, e.g., Tylenol represents all medicines that contain acetaminophen, pseudoephedrine hydrochloride, dextromethorphan hydrobromide and chlorpheniramine maleate. Due to space constraints, more normalization of diseases and medications could be found in our repository⁶.

B Experiments

B.1 Baselines

- TF-IDF. This is a traditional bag-of-word model for text classification. We view each dialogue as text and the corresponding medication as label, and train a classification model based on TF-IDF features of words.
- LSTM-flat. This is a LSTM-based method. It concatenates all the sentences in a dialogue as a long sentence and feeds the long sentence into the BiLSTM to get the dialogue embedding for medication prediction.
- LSTM-hier. This is also a LSTM-based method. Different from LSTM-flat, it uses a hierarchical BiLSTM where each word in an utterance are fed into BiLSTM to get the utterance embedding and then the utterances are fed into another BiLSTM to get the final dialogue embedding. It captures both word-level and utterance-level dependencies.
- **RETAIN**. This is a RNN-based EHR medication recommendation method using on a two-level neural attention network that detects influential past visits. In the current scenario, it is used to model the dialogues.
- DAG-ERC. This method designed a directed acyclic neural network to model the information flow between long-distance conversation background and nearby context. Following the implementation in (Shen et al., 2021b), the features of utterances extracted from finetuning RoBERTa are inputted in model while the model structure is RNN based, so DAG-ERC is regraded as a RNN-based model.
- **HiTANet**. This is a Transformer-based risk prediction approach on EHR, which model time information in local and global stages. We transform this method to model the hidden temporal information in medical dialogues.
- LSAN. This is also a Transformer-based risk prediction approach, to model the hierarchical structure of EHR data. We modified this

⁶https://github.com/Hhhhhhhzf

method to model the hierarchical structure in medical dialogues and add disease module of DDN to encoder the external knowledge.

- **DialogXL**. This method improves XLNet with enhanced memory and dialog-aware self-attention. We modify the softmax layer to sigmoid layer in this model to fit the multilabel task in medication recommendation and add the disease module of DDN.
- DDN. This is our proposed model. It utilizes
 the dialogue structure and external disease
 knowledge to enhance the dialogue-based
 medication recommendation performance.

B.2 Evaluation Metrics

Jaccard =
$$\frac{1}{|D|} \sum_{k=1}^{|D|} \frac{|Y^{(k)} \cap \hat{Y}^{(k)}|}{|Y^{(k)} \cup \hat{Y}^{(k)}|}$$
(9)

$$F1 = \frac{1}{|D|} \sum_{k=1}^{|D|} \frac{2 \cdot P^{(k)} \cdot R^{(k)}}{P^{(k)} + R^{(k)}}$$
(10)

where |D| is the number of dialogues in the test set. $Y^{(k)}$ represents the ground truth medication set of the kth dialogue, and $\hat{Y}^{(k)}$ represents the predicted medication set of the kth dialogue by the model. $P^{(k)}$, $R^{(k)}$ represents the Precision and Recall of the kth dialogue, respectively.

B.3 Additional Experiment on DDI

Medication combination recommendation would trigger the Drug-Drug Interaction (**DDI**) inevitably, which might lead to adverse outcomes. To this end, we explore the DDI in DIALMED. And we follow the previous work (Shang et al., 2019b) to give the DDI rate definition (smaller value means better).

$$DDIRate = \frac{\sum_{k}^{N} \sum_{i,j} |\{(c_i, c_j) \in \hat{Y}^{(k)} | (c_i, c_j) \in \mathcal{E}_d\}|}{\sum_{k}^{N} \sum_{i,j} 1}$$
(11)

where the set will count each medication pair (c_i, c_j) in recommendation set \hat{Y} if the pair belongs to edge set \mathcal{E}_d of the DDI graph. Here N is the size of test dataset. In addition, DDI relationships among medications in DIALMED are collected from YAOZH 7 , a medical data retrieval system.

The evaluation results are shown in Table 5. We could find that ground truth DDI rate is very small (compared to the 8.08% in MIMIC-III (Yang

et al., 2021)), which may lead to the low rate on models. In view of this situation, we think it is no need for additional efforts to control the DDI rate at the current stage. Considering for the future research, we open source our DDI relationship graph in our repository.

		DDI Rate				
Model	All Data	Respiratory	Gastroenterology	Dermatology		
G.T.	1.12	0.78	2.06	0.74		
TF-IDF	1.10	0.46	2.01	0.51		
LSTM-flat	0.58	1.36	0.93	0.00		
LSTM-hier	1.02	0.11	0.91	0.65		
RETAIN	1.92	1.12	1.89	0.00		
DAG-ERC	0.81	1.01	1.53	0.48		
HiTANet	0.45	1.49	1.09	0.50		
LSAN	1.57	0.00	1.62	0.48		
DialogXL	1.34	1.09	1.59	0.40		
DDN	1.90	0.20	1.54	0.47		

Table 5: DDI Rate (%) comparison on DIALMED. G.T. represents the Ground Truth.

C Task

C.1 Medical Utility

Medical treatment includes a number of steps: registration, examination, image reading, report interpretation, diagnosis, prescription and so on. AI medicine could help optimize resource allocation and improve efficiency in all aspects of health care. To this end, there are two kinds of computer aided diagnosis system, image diagnosis and text diagnosis. Due to the higher threshold of diagnosis, current researches are more inclined to image analysis, and there is still a lot of room for development in text diagnosis. Conversations in outpatient clinics are not reserved and involved many severe data privacy implications, leading to dialogue-based drug recommendation mainly oriented to telemedicine. The medical dialogue system, as a assistant of doctors, could give auxiliary medication suggestions based on the contexts when doctors and patients are communicating with each other.

D Statistics

D.1 Ratio of consulting for medications

The ratio of the patients to consult for medications is calculated with regular expressions. In the first place, 10,0000 different medical conversations from our dialogue corpus based on random sampling are fetched. For every dialogue, we apply the regular expression (e.g., "[Ww]hat (medication|drug|medicine) should I (take|eat)") on the utterances spoken by the patient and assume

⁷https://db.yaozh.com/interaction

that it is a case of consulting for drugs if the regular expression matches. The regular expressions are collected based on our observation and understanding of data. More regular expressions could be found in our repository.

D.2 Complete Corpus Statistics

The frequency of all diseases and medications is shown in Figure 7 & 8.

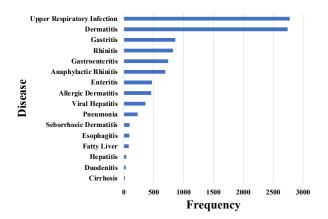


Figure 7: The frequency of all diseases.

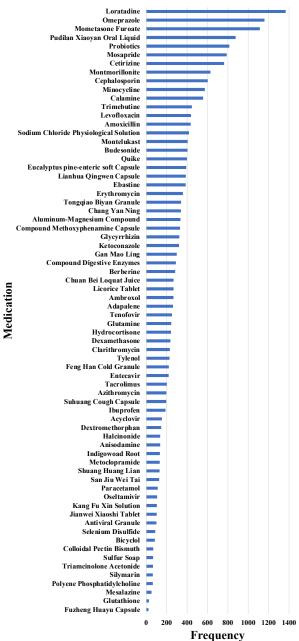


Figure 8: The frequency of all medications. The names are translated from Chinese.