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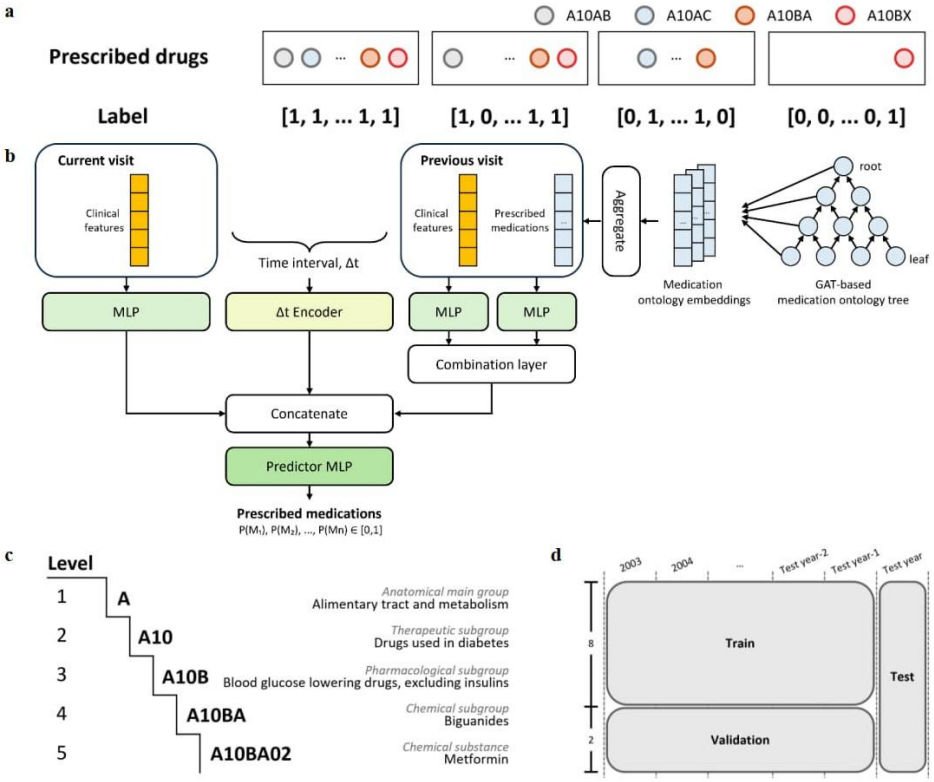
AI-Based Medication Recommendation for Diabetic Kidney Disease: Robust to Temporal Data Shifts and New Drugs

Seoyoung Choi[1], Hyoju Sohn[4], Jinyeong Yi[4], Myeongju Kim, Seokwoo Park[3], Sejoong Kim[3]
[1]Department of Medicine, Seoul National University College of Medicine, Korea, Republic of
[2]Department of Center for Artificial Intelligence in Healthcare, Seoul National University Bundang Hospital, Korea, Republic of
[3]Department of SickGPT Inc., SickGPT Inc., Korea, Republic of
[4]Department of Internal Medicine-Nephrology, Seoul National University Bundang Hospital, Korea, Republic of

Objectives : Medication management in diabetic kidney disease (DKD) is clinically complex. Although AI–based medication recommendation models have shown promise using electronic health records (EHR), their real-world applicability under changes in clinical environment during deployment—such as the introduction of new medications, evolving prescribing guidelines, and changes in patient population characteristics —remains unclear. We developed an AI-based medication recommendation model for DKD patients designed to be robust to temporal shifts and extensible to novel medications by utilizing clinical features and ATC ontology-based embeddings.
Methods : Based on EHR data between 2003 and 2017, we developed a multilabel prediction model predicting level-4 ATC codes from demographic, laboratory, and medication histories, with medication embeddings learned via a graph attention network over the ATC ontology. To simulate real-world deployment, the model was trained cumulatively by year and evaluated on the subsequent year. Performance (PRAUC, F1, Jaccard) and hierarchical generalization to newly introduced drugs were evaluated.
Results : Model performance improved rapidly as the training window expanded from 2003–2004 to 2003–2009, followed by more gradual gains thereafter. Performance plateaued beginning with the 2010 test year at approximately PRAUC 0.881, F1 0.785, and Jaccard 0.743, and remained stable across subsequent evaluation years. For newly introduced medications in the test year, evaluation at the parent-level (ATC level-3) yielded performance comparable to that of medications observed during training.
Conclusions : In this study, we developed and evaluated an AI-based medication recommendation model for DKD that addresses key challenges in real-world clinical deployment by integrating clinical features with ATC ontology–based embeddings. We showed that the model can provide informative higher-level recommendations when encountering previously unseen drugs and maintains stable performance across temporal data shifts when trained with sufficient longitudinal data. These findings suggest that combining patient clinical features with medication ontology representations enables stable and practically useful AI-based medication recommendations for chronic diseases under evolving clinical environments.

Figure 1.jpg

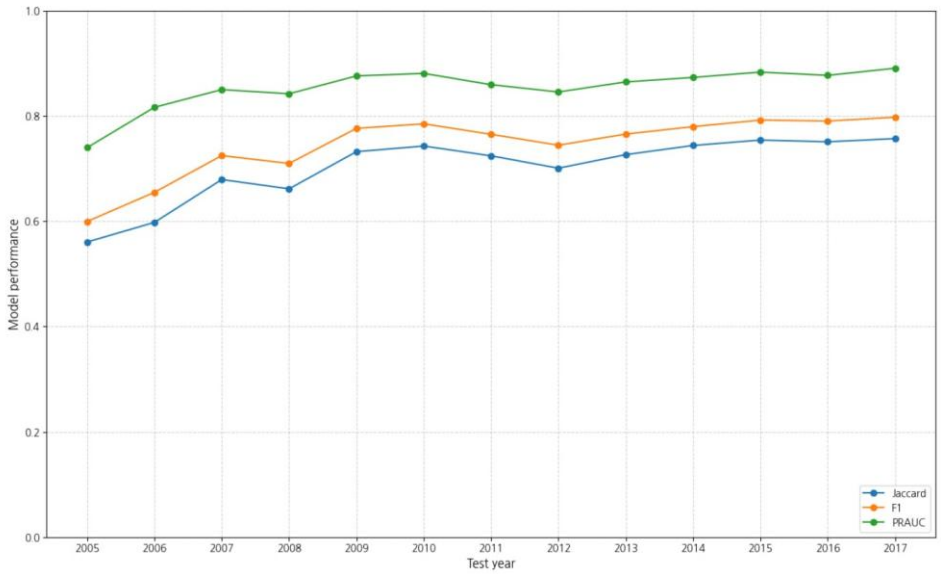
Figure 1. Overview of the study



a. Medication recommendation task description; **b.** Framework of the medication recommendation; **c.** Hierarchical ontology structure of the ATC code; **d.** Train, validation and evaluation scheme

Figure 1.jpg

Figure 2. Performance trends by the year



Note. Area Under the Precision-Recall Curve, PRAUC