MLKD 2024
The First International Conference on
Machine Learning and Knowledge Discovery
Amirkabir University of Technology, December 18-19, 2024

Optimizing Drug-Disease Association Analysis: A Resource-Efficient Approach Using Numerical Linear Algebra and Machine Learning

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Abstract

In today's data-driven world, the growing volume of information demands the development of models that balance accuracy and computational efficiency. Drug repurposing has emerged as a pivotal strategy in the pharmaceutical industry, enabling the identification of new therapeutic uses for existing drugs. However, with the increasing amount of available data, it is essential for researchers and industry stakeholders to create models that maintain predictive accuracy while minimizing computational costs. Our study builds on the state-of-the-art WNMFDDA (Weighted Graph Regularized Collaborative Non-negative Matrix Factorization for Drug-Disease Association Prediction) model, which is known for its high predictive accuracy. We focus on optimizing this approach by significantly reducing memory usage and computational time, achieving an 8-fold reduction in time cost and over a 400-fold decrease in storage cost during model training, all without compromising accuracy. Our findings show that several alternative methods can deliver performance metrics close to the reference model while substantially lowering both memory and computational requirements. This approach not only retains the accuracy of drug-disease association predictions but also enhances the efficiency of the drug repurposing process, enabling quicker transitions from research to clinical applications. By optimizing computational resources, this work provides a scalable and efficient solution for future drug discovery and repurposing efforts.

Keywords: Drug Repurposing, Machine Learning, Numerical Linear Algebra, Drug-Disease Association, Non-negative matrix factorization

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