Automatically classifying study designs of biomedical literature relevant for inclusion in the Drug Interactions Knowledge Base

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A longstanding issue with knowledge bases that discuss drug-drug interactions (DDIs) is that they are inconsistent with one another. One potential reason is that experts might vary in their approach to assessing the evidence about potential DDIs. We think that a particularly promising future research direction would be computerized decision support to help experts be more objective in these assessments. In the current study, we tested the feasibility of using machine learning in conjunction with an ontology called DIDEO—the Potential Drug-drug Interaction and Potential Drug-drug Interaction Evidence Ontology—to automatically classify the evidence types of clinical DDI studies.

The evidence type component of the DIDEO ontology provides definitions of 44 different evidence types relevant for establishing DDIs and specifies the necessary conditions for each one [DIDEO Ontology, 2014; Utecht et al., 2017]. Our current experiments focused on distinguishing six of these evidence types using five sub-classifiers divided into three levels based on DIDEO’s hierarchy of evidence. Each sub-classifier was a support vector machine trained using 5-fold cross validation and a class weighting mechanism. Reference set data came from a dataset that contains 189 full text clinical DDI studies annotated for their evidence types (i.e., study designs). We derived unigram features from the titles, abstracts, and methods sections of the full text studies.

The sub-classifiers were evaluated using AUROC, precision (P), recall (R) and F1. The weighted average of all the sub-classifiers was AUROC = 0.91, P = 0.90, R = 0.91 and F1 = 0.89. Sub-classifiers’ prediction performance is shown in the figure. In another evaluation, we ran the hierarchical classifier as a whole on a held-out dataset of 32 studies. The classifier predicted correctly 27/32 articles (84% accuracy) compared with an expert’s judgment. The weighted average of all the sub-classifiers for the held-out dataset was P = 0.95; R = 0.98.

The results show that our approach of using a hierarchical study type classifier scheme based on evidence types in the DIDEO ontology is promising. In the future, such an automatic classification system could be a key component of a computerized decision support to help experts be more objective in DDI evidence assessment, ultimately assisting drug compendium editors as they assess evidence items. Other promising applications of the technology would be to support automatic identification of new clinical DDI studies, and to help extend the DIDEO ontology to new evidence sub-types.

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References