

Exploring Pattern Structures of Syntactic Trees for Relation Extraction

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Task: Drug-Drug Interaction (DDI) Extraction


Given a sentence, where the drugs are (automatically) annotated, find the pairs of drugs that interact.

Antihistamines may enhance the effects of **tricyclic antidepressants**, **barbiturates**, **alcohol**, and other **CNS depressants**.



The diagram illustrates drug-drug interactions (DDI) in the sentence above. Blue arcs connect 'Antihistamines' to 'tricyclic antidepressants', 'barbiturates', and 'CNS depressants'. A red arc connects 'barbiturates' and 'alcohol'.

ZEBETA should not be combined with other **beta-blocking agents**.



The diagram illustrates a drug-drug interaction (DDI) in the sentence above. A blue arc connects 'ZEBETA' and 'beta-blocking agents'.

Methods in DDI Extraction

Ensemble Learning (P. Thomas et al. 2011)

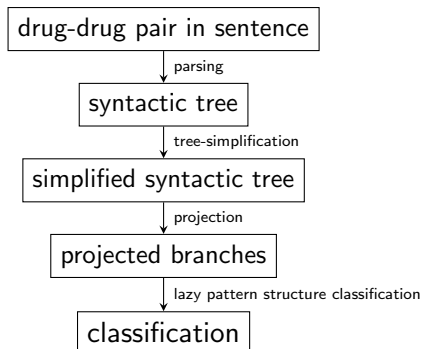
Combination of different kernel based systems (majority voting):

- all-paths graphs (dependency trees)
- k-band shortest path (dependency trees)
- shallow linguistic features

Cased based Reasoning (Maora):

- Each pair is represented by a context and a set of features (lemma, POS, roles)

Pipeline of our approach



The DDI Dataset

The dataset used, is of the DDI extraction challenge 2011.¹

- Build from Drugbank articles
- Drugs are tagged automatically
- Interactions are extracted from the DrugBank, and were manually checked by two domain experts
- Around 4.000 sentences, containing around 2.300 positive and 20.000 negative interactions.

¹<http://labda.inf.uc3m.es/DDIExtraction2011/dataset.html>

Entity blinding

- Drugs of the drug-drug pair are replaced with 'drug_tag_r'
- Other drugs are replaced with 'drug_tag'

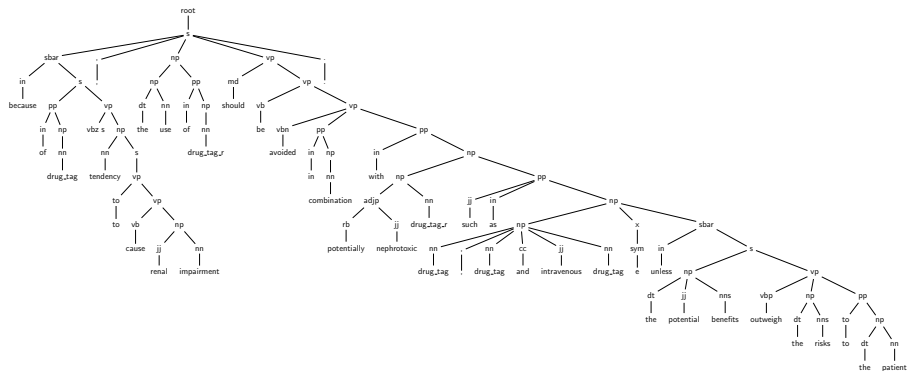
*Because of **foscarnets** tendency to cause renal impairment, the use of **FOS-CAVIR** should be avoided in combination with potentially **nephrotoxic drugs** such as **aminoglycosides**, **amphotericin B** and **intravenous pentamidine** unless the potential benefits outweigh the risks to the patient.*

*Because of **drug_tag** tendency to cause renal impairment, the use of **drug_tag_r** should be avoided in combination with potentially **drug_tag_r** such as **drug_tag**, **drug_tag** and **drug_tag** unless the potential benefits outweigh the risks to the patient.*

Then the syntax tree is constructed (Stanford Constituency Parser)

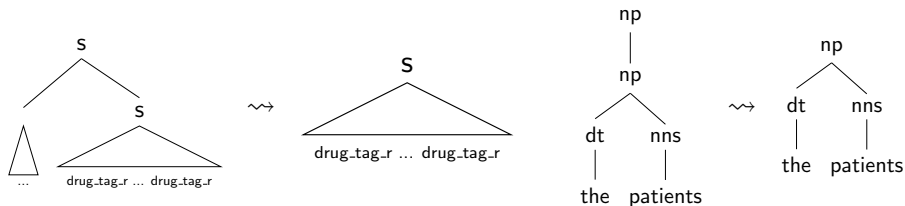
Size of Syntactic Trees

Contains 122 nodes (130 on average, 311 max)



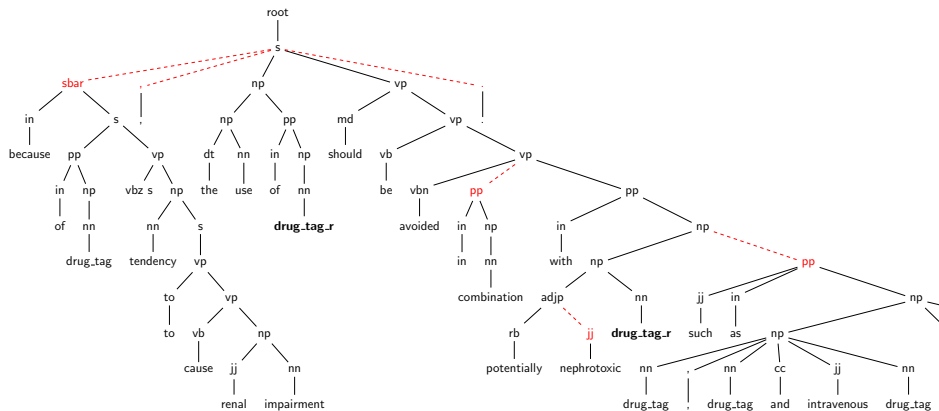
Tree Simplification

- 1 Removal of JJ, PP, S, SBAR, PRN subtrees that don't contain 'drug_tag_r'
- 2 VP-nodes become NEGVP if they contain a negation.
- 3 Only the lowest S node containing both 'drug_tag_r' tags is considered.
- 4 Contraction of non-branching trees



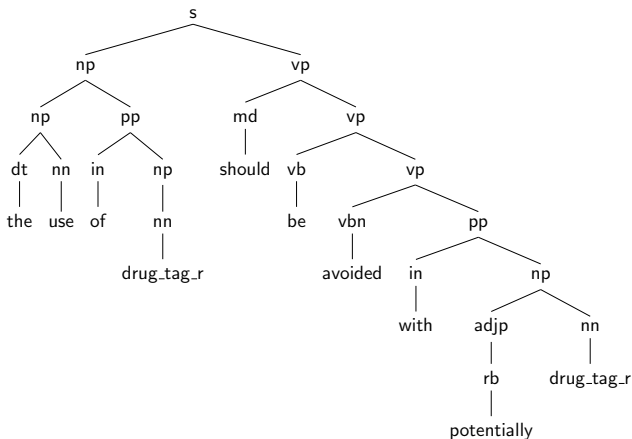
¹ JJ=adjective, PP=prepositional phrase, S/SBAR=sentence, PRN=bracketed expression, VP=verb phrase

Simplifications



Simplified Tree

Contains 31 nodes (41 on average, 138 max)



Pattern Structures (B. Ganter and S. Kuznetsov 2001)

A *pattern structure* is defined as a tuple $(G, (D, \sqcap), \delta)$

- G is the set of objects
- D is the set of object descriptions (or patterns)
- $\delta : G \rightarrow D$ maps objects to their corresponding description
- \sqcap is a similarity operator on subsets of D (idempotent, associative, and commutative)

The subsumption relation between subsets of descriptions can be defined in a standard way:

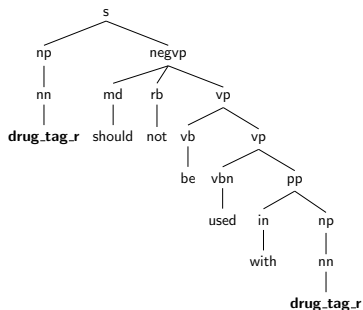
$$A \sqsubseteq B :\Longleftrightarrow A \sqcap B = A$$

Pattern Structure of Syntactic Trees $(G, (D, \sqcap), \delta)$

Object

Anafranil should not be used with **MAO inhibitors**. (d16.s2.p0)

Object Description

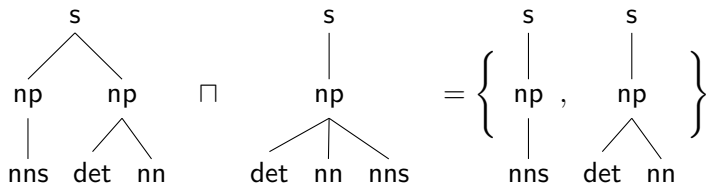


Pattern Structure of Syntactic Trees $(G, (D, \sqcap), \delta)$

Rooted Tree Intersection (\sqcap)

The *Rooted Intersection* between tree t_1 and tree t_2 is the set of maximal trees from the intersection of all rooted subtrees of t_1 and those of t_2 .

Example



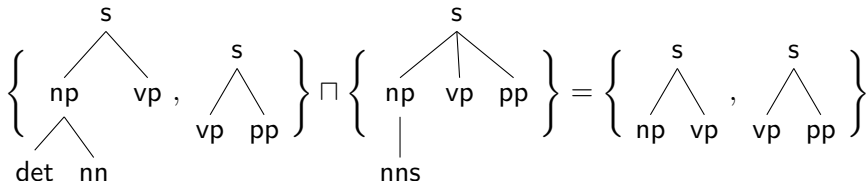
Pattern Structure of Syntactic Trees $(G, (D, \sqcap), \delta)$

Similarity Operator (\sqcap)

The *similarity* between a set of trees A and a set of trees B ($A \sqcap B$) is the set of maximal trees from

$$\bigcup_{(t_a, t_b) \in A \times B} t_a \sqcap t_b$$

Example

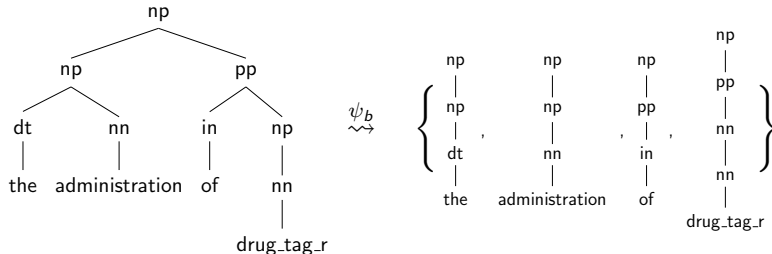


Projection for the Pattern Structure of Syntactic Trees

Branch Projection

The branch projection of a tree t is the set of its branches $\psi_b(t)$.

Example

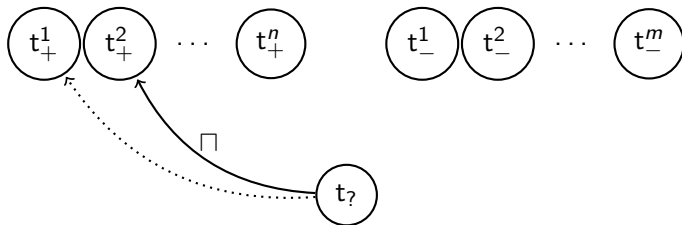


Lazy Pattern Structure Classification (Kuznetsov 2013)

Given:

- set of positive examples T_+
- set of negative examples T_-

A new object $t_?$ is classified as positive iff a positive hypothesis can be found in T_+ .

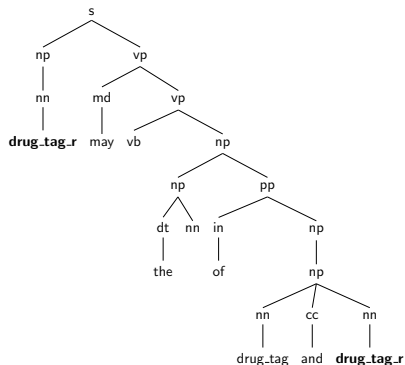


$$\exists t_+ \in T_+ \quad \forall t_- \in T_- : (\delta(t_?) \sqcap \delta(t_+)) \not\sqsubseteq \delta(t_-)$$

Example of a Positive Hypothesis

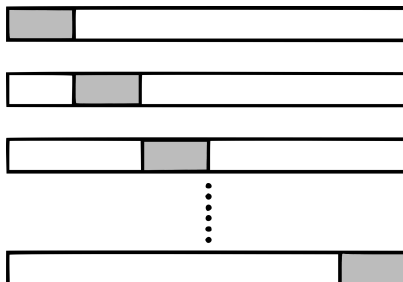
t_- : **Ketoconazole** tablets may alter the metabolism of cyclosporine, tacrolimus, and **methylprednisolone**, resulting in elevated plasma concentrations of the latter drugs.

t_+ : **Ethoxzalamide** may increase the action of tricyclics, amphetamines, **procainamide**, and quinidine.



10-fold Cross Validation

We did a 10-fold cross validation on the 23.000 drug-drug pairs.



We calculate precision, recall and f-measure over all the folds.

Results

Simplifications	P	R	F ₁
1. NEGVP, contraction	0.32	0.39	0.35
2. lowest-S, contraction	0.27	0.49	0.35
3. NEGVP, lowest-S	0.36	0.45	0.38
4. NEGVP, lowest-S, contraction	0.30	0.49	0.37
5. NEGVP, lowest-S, vp-map	0.35	0.45	0.39
6. NEGVP, lowest-S, vp-map, prep-map	0.39	0.41	0.40

Table: Results from 10-fold cross validation on the DDI 2011 data set. Performance is measured in precision (P), recall (R) and F₁-measure (F₁). In all conditions constituent simplification is applied.

Error Analysis

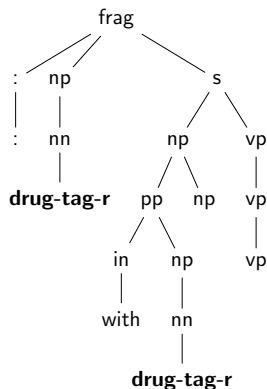
Error categories that we found:

- Non-sentences (NP, FRAG)
- Very deep syntactic trees (mostly FN)
- Mistakes in annotation (mostly FP)
- Insufficient similarity
- Parsing errors

False Positive

$t_?$: **Thalidomide**: Co-administration with **thalidomide** should be employed cautiously, as toxic epidermal necrolysis has been reported with concomitant use.

t_+ : **Corticosteroids**: Concomitant administration with **aspirin** may increase the risk of gastrointestinal ulceration and may reduce serum salicylate levels



Conclusions & Future Work

Proposed:

- Pattern structure of syntactic trees
- Branch-projection
- Extraction of characteristic syntactic tree patterns for classification

Future work:

- Filter badly performing patterns
- Use the patterns in different classification paradigms
- Improve the tree simplifications
- Include morphological or semantic information in the trees
- Application to dependency graphs, or parse thickets

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False Positive

test: It is not known if **hormonal contraceptives** differ in their effectiveness when used with **Accutane.**

