

# Master in Artificial Intelligence

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

## Advanced Human Language Technologies



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# Outline

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

1 DDI Baseline

2 General Structure

3 Resources

4 Core task

5 Goals & Deliverables

# Session 3 - DDI baseline

## Assignment

### DDI Baseline

#### General Structure

#### Resources

#### Core task

#### Goals & Deliverables

The main program parses all XML files in the folder given as argument and classifies drug-drug interactions between pairs of drugs. The program must use **simple heuristic rules** to carry out the task.

```
$ python3 ./baseline-DDI.py data/Devel/  
DDI-DrugBank.d278.s0|DDI-DrugBank.d278.s0.e0|DDI-DrugBank.d278.s0.e1|null  
DDI-MedLine.d88.s0|DDI-MedLine.d88.s0.e0|DDI-MedLine.d88.s0.e1|null  
DDI-MedLine.d88.s0|DDI-MedLine.d88.s0.e0|DDI-MedLine.d88.s0.e2|null  
DDI-MedLine.d88.s0|DDI-MedLine.d88.s0.e1|DDI-MedLine.d88.s0.e2|null  
DDI-DrugBank.d398.s0|DDI-DrugBank.d398.s0.e0|DDI-DrugBank.d398.s0.e1|effect  
DDI-DrugBank.d398.s0|DDI-DrugBank.d398.s0.e0|DDI-DrugBank.d398.s0.e2|effect  
DDI-DrugBank.d398.s0|DDI-DrugBank.d398.s0.e2|DDI-DrugBank.d398.s0.e3|null  
DDI-DrugBank.d398.s1|DDI-DrugBank.d398.s1.e0|DDI-DrugBank.d398.s1.e1|null  
DDI-DrugBank.d211.s2|DDI-DrugBank.d211.s2.e0|DDI-DrugBank.d211.s2.e5|mechanism  
DDI-DrugBank.d211.s2|DDI-DrugBank.d211.s2.e1|DDI-DrugBank.d211.s2.e2|null  
...
```

# Outline

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

1 DDI Baseline

2 General Structure

3 Resources

4 Core task

5 Goals & Deliverables

# General Structure - Main function

```
# process each file in directory
for f in listdir(datadir) :
    # parse XML file, obtaining a DOM tree
    tree = parse(datadir + "/" + f)
    # process each sentence in the file
    sentences = tree.getElementsByTagName("sentence")
    for s in sentences :
        sid = s.attributes["id"].value # get sentence id
        stext = s.attributes["text"].value # get sentence text

        # load sentence entities into a dictionary
        entities = {}
        ents = s.getElementsByTagName("entity")
        for e in ents :
            eid = e.attributes["id"].value
            entities[eid] = e.attributes["charOffset"].value.split("-")

        # Tokenize, tag, and parse sentence
        analysis = deptree(stext)

        # for each pair in the sentence, decide whether it is DDI and its type
        pairs = s.getElementsByTagName("pair")
        for p in pairs:
            id_e1 = p.attributes["e1"].value
            id_e2 = p.attributes["e2"].value
            ddi_type = check_interaction(analysis, entities, id_e1, id_e2)
            if ddi_type != None :
                print(sid+"|"+id_e1+"|"+id_e2+"|"+ddi_type], file=outf)

# get performance score
evaluator.evaluate("DDI",inputdir,outputfile)
```

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

# Outline

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

1 DDI Baseline

2 General Structure

3 Resources

4 Core task

5 Goals & Deliverables

# Resources

DDI Baseline

General  
Structure

Resources

Core task

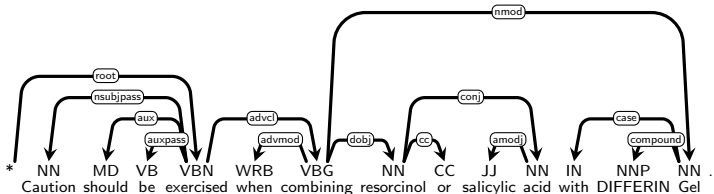
Goals &  
Deliverables

We will use Stanford CoreNLP dependency parser, which can be called via `nltk`, and integrates a [tokenizer](#), a [part-of-speech](#) tagger, and a [dependency parser](#).

- Download and uncompress [Stanford CoreNLP](#).
- Provided class `deptree.py` will handle calling the parser and access the resulting structure

# Functions - Analyze text

```
text = 'Caution should be exercised when combining resorcinol or  
       salicylic acid with DIFFERIN Gel'  
analysis = deptime(text)  
analysis.get_word(tk)  
analysis.get_lemma(tk)  
analysis.get_tag(tk)  
analysis.get_rel(tk)  
analysis.get_parent(tk)  
analysis.get_children(tk)  
analysis.get_ancestors(tk)  
analysis.get_up_path(tk1,tk2)  
...
```



DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables



# Functions - Check for Drug-Drug Interactions

```
def check_interaction(analysis,entities,e1,e2) :  
    ,,,
```

Task:

Decide whether a sentence is expressing a DDI between two drugs.

Input:

analysis: a DependencyGraph object with all sentence information  
entities: A list of all entities in the sentence (id and offsets)  
e1,e2: ids of the two entities to be checked.

Output: Returns the type of interaction ('effect', 'mechanism', 'advice', 'int') between e1 and e2 expressed by the sentence, or 'None' if no interaction is described.

```
    ,,,
```

```
# get head token for each gold entity
```

```
tkE1 = tree.get_fragment_head(entities[e1]['start'],entities[e1]['end'])  
tkE2 = tree.get_fragment_head(entities[e2]['start'],entities[e2]['end'])
```

```
p = patterns.check_LCS_svo(tree,tkE1,tkE2)  
if p is not None: return p
```

```
p = patterns.check_wib(tree,tkE1,tkE2,entities,e1,e2)  
if p is not None: return p
```

```
## add more patterns to improve performance  
# p = patterns.check_XXXX(tree,tkE1,tkE2,...)  
# if p is not None: return p
```

```
return "null"
```

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

# Predefined Functions - Evaluation

Performance evaluation functions are available in module evaluator, so you need to add to your main program

```
from evaluator import evaluate
```

The behaviour and parameters of evaluate are:

```
def evaluate(task, datadir, outfile) :  
'''
```

Task:

Compare results in outfile with ground truth annotations in datadir, and produce performance statistics.

Input:

task: string with the name of the task to evaluate: "NER" or "DDI"  
datadir: directory containing original XML files with the ground truth  
outfile: filename containing the entities produced by your system

Output:

Stats table about the predicted entities in the given output file  
'''

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

# Outline

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

- 1 DDI Baseline
- 2 General Structure
- 3 Resources
- 4 Core task
- 5 Goals & Deliverables

# Detecting interactions - First baseline

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

Function `check_interaction` will implement our *simple* rule-based interaction detector.

- It is a *baseline*, i.e. a lower bound for the performance of ML systems that we will build later.
- It must consist of an *if-then-else* cascade of *simple* rules. Do not implement statistical approaches.

# Detecting interactions - Choosing the rules

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

- Examine (by hand or collecting simple statistics) the **train** dataset and try to infer general rules that are right in most cases, even if they seldom apply (high precision, low recall).
- Express your observations in terms of *if-then-else* rules. Note that the order in which the rules are checked will alter the results, so you should apply first those rules with higher precision.
- Use the **train** dataset to make your observations. Use provided program `explore.py` to implement a new rule and get an idea of its potential utility

# Detecting interactions - Initial rules

The initial version of `baseline-DDI.py` has two rules, based on the following explorations:

- When the two target entities are one under the subject (`nsubj`) and the other under the direct object (`obj`) of a verb, then it is likely that there is an interaction. Some verbs will be indicative of certain relations.

Pattern `check_LCS_svo` in `patterns.py` spots trees with this structure, and check for some relevant verbs

- Tree structure is not matched often. A more relaxed pattern could be checking whether certain words appear in between both entities.

Pattern `check_wib` in `patterns.py` checks whether certain words appear in between the two target entities.

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

# Detecting interactions - Improving the rules

## Suggestions to improve performance

- Use program `explore.py` to get possible words to add to the lists in existing patterns `check_LCS_svo` and `check_wib`.
- Identify weak classes in your predictor (e.g. class `advise` has very low recall) and try to identify patterns that could help improving them.

E.g. Using `explore.py` to find examples of class `advise`, we see that the main verb is very often modified with *should*. Try adding a pattern in `patterns.py` that checks whether the LCS of both entities is a verb with a *should* child, and return 'advise' if it is.

- Identify other weak spots (e.g. `mechanism` has low recall) and try to figure out some patterns that could help improving that class.

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

# Outline

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

1 DDI Baseline

2 General Structure

3 Resources

4 Core task

5 Goals & Deliverables



# Exercise Goals

What you should do:

- Derive simple rules from data observation (using `explore.py` may be helpful)
- Create a *simple* baseline for DDI using an *if-then-else* sequence of patterns rules.

What you should **NOT** do:

- Apply statistical algorithms or weighted information combination that are not a cascade of *if-then-else* rules.
- Try too hard: The goal is to calibrate the difficulty of the task, seeing how far can we get with *little effort*.  
**However:** This task is not as easy as NER, and the code checking the applicability of the rules will be more complex. Maintain the structure of provided `check_interaction` function, just adding new patterns (which should be in `patterns.py`)

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

# Exercise Goals

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

## Orientative results:

- Provided initial version achieves 30% macro average F1 on devel with two rules.
- Improve/extend the rule set to achieve 35%-40% macro average F1 on devel (see suggestions on previous slides)

# Deliverables

DDI Baseline

General  
Structure

Resources

Core task

Goals &  
Deliverables

- You'll be expected to produce a report at the end of DDI task.
- By now, just keep track of the information you'll need later:
  - Observations drawn from the data
  - Rules build from those observations
  - Rules tried and discarded/kept
  - Performance results on devel and test corpus using different rule combinations