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### Session 3 - DDI baseline

### Assignment

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Write a python program that 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|0|null DDI-MedLine.d88.s0|DDI-MedLine.d88.s0.e0|DDI-MedLine.d88.s0.e1|0|null DDI-MedLine, d88, s0 DDI-MedLine, d88, s0, e0 DDI-MedLine, d88, s0, e2 0 null DDI-MedLine, d88, s0 DDI-MedLine, d88, s0, e1 DDI-MedLine, d88, s0, e2 0 null DDI-DrugBank.d398.s0|DDI-DrugBank.d398.s0.e0|DDI-DrugBank.d398.s0.e1|1|effect DDI-DrugBank.d398.s0|DDI-DrugBank.d398.s0.e0|DDI-DrugBank.d398.s0.e2|1|effect DDI-DrugBank.d398.s0|DDI-DrugBank.d398.s0.e2|DDI-DrugBank.d398.s0.e3|0|null DDI-DrugBank.d398.s1|DDI-DrugBank.d398.s1.e0|DDI-DrugBank.d398.s1.e1|0|null DDI-DrugBank.d211.s2/DDI-DrugBank.d211.s2.e0/DDI-DrugBank.d211.s2.e5/1/mechanism DDI-DrugBank.d211.s2|DDI-DrugBank.d211.s2.e1|DDI-DrugBank.d211.s2.e2|0|null

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### General Structure - Main function

```
# process each file in directory
for f in listdir(inputdir) :
   # 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 :
         id = e.attributes["id"].value
         offs = e.attributes["charOffset"].value.split("-")
         entities[id] = offs
      # Tokenize, tag, and parse sentence
      analysis = analyze(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
         (is_ddi_ddi_type) = check_interaction(analysis, entities, id_e1, id_e2)
         print("|".join([sid, id_e1 id_e2, is_ddi, ddi_type]), file=outf)
# get performance score
evaluate(inputdir.outputfile)
```

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### Resources

You will need to use a tokenizer, a part-of-speech tagger, a dependency parser.

We recommend Stanford CoreNLP dependency parser, which can be called via nltk, and integrates all three steps. (You'll need to add token spans, though):

**1** Download and uncompress Stanford CoreNLP.

2 Launch a CoreNLP server: cd stanford-corenlp-full-2018-10-05 java -mx4g -cp "\*" edu.stanford.nlp.pipeline.StanfordCoreNLPServer 3 In your python program: # import nltk CoreNLP module (just once) from nltk.parse.corenlp import CoreNLPDependencyParser # connect to your CoreNLP server (just once) my.parser = CoreNLPDependencyParser(url="http://localhost:9000") # parse text (as many times as needed) mytree, = my\_parser.raw\_parse(mytext)

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### Functions - Analyze text

### def analyze(s) :

- Input: Receives a sentence text s, and sends it to CoreNLP to obtain the tokens, tags, and dependency tree. It also adds the start/end offsets to each token
- Output: Returns the nltk DependencyGraph object produced by CoreNLP, enriched with token offsets.

### Example:

>>> analyze("Caution should be exercised when combining resorcinol or salicylic acid with DIFFERIN Gel")  $\,$ 

```
{0:{'head':None,'lemma':None,'re1':None,'tag':'TOP','word':None},
1:{'word':'Caution','head':4,'lemma':'caution','re1':'aux,'htag':'MD','start':8,'end':16},
2:{'word':'be','head':4,'lemma':'bould','re1':'aux,'tag':'WE','start':15,'end':16},
3:{'word':'be','head':4,'lemma':'exercise','re1':'Auxpass','tag':'VE','start':15,'end':16},
4:{'word':'when','head':6,'lemma':'exercise','re1':'Auxpass','tag':'VE','start':15,'end':16},
5:{'word':'when','head':6,'lemma':'centrise','re1':'auxpass','tag':'VE','start':28,'end':16},
6:{'word':'when','head':6,'lemma':'centrise','re1':'advond','tag':'VE','start':33,'end':16},
6:{'word':'resorcino1','head':6,'lemma':'combine','re1':'advc1','tag':'VE','start':33,'end':16},
9:{'word':'resorcino1','head':6,'lemma':'centrise','re1':'advc1','tag':'VE','start':43,'end':15},
9:{'word':'salicylic','head':10,'lemma':'salicylic','re1':'amod','tag':'JJ','start':57,'end':76,'
11:{'word':'with','head':13,'lemma':'DIFFERIN','re1':'compound','tag':'NN','start':75},
12:{'word':'Gel','head':6,'lemma':'DIFFERIN','re1':'compound','tag':'NN','start':75},'
13:{'word':'Gel','head':6,'lemma':'DIFFERIN','re1':'compound','tag':'NN','start':75,'end':76},'
13:{'word':'Gel','head':6,'lemma':'Compound','tag':'NN','start':75,'end':76},'
13:{'word':'Gel','head':6,'lemma':'Compound','tag':'NN','start':75,'end':76},'
14:{'word':'Gel','head':6,'lemma':'DIFFERIN','re1':'rompound','tag':'NN','start':75,'end':76},'
14:{'word':'Gel','head':6,'lemma':'DIFFERIN','re1':'rompound','tag':'NN','start':75,'end':76},'
14:{'word':'Gel','head':6,'lemma':'Compound','tag':'NN','start':75,'end':76},'
14:{'word':'Gel','head':6,'lemma':'Compound','tag':'NN','start':75,'end':76},'
14:{'word':'Gel','head':6,'lemma':'Compound','tag':'NN','end':75,'end':76},'
14:{'word':'Compound':'Compound','tag':'NN','gel':'NN','ga','Compound','tag':'NN','ga','Compound','tag':'NN','ga','Compound','tag':'NN','ga','Compound','tag':'NN','ga','Compound','tag':'NN','ga','Compound','tag','Compound','tag':'NN','ga','Compound','tag','Compound','tag','Comp
```

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#### Functions - Analyze text DDI Baseline (nmod) General Structure (root) Resources nsubjpass COR Detailed advcl case Structure advmod amod compound auxpass Core task NN MD VB ŇΒΝ WRB ŮВĞ NŇ CC JJ ŇΝ IN NNP ŇΝ Caution should be exercised when combining resorcinol or salicylic acid with DIFFERIN Gel Evaluating Results

### Functions - Check for Drug-Drug Interactions

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Evaluating Results def check\_interaction(analysis,entities,e1,e2) :

- Input: Receives a DependencyGraph object with all sentence information, a list of all entities in the sentence (id and offsets), and the ids of the two entities to be checked.
- Output: Returns a 0/1 value indicating whether the sentence states an interaction between entities e1 and e2, and the type of interaction (null if there is none).

### Functions - Evaluation

def evaluate(inputdir, outputfile) :

- Input: Receives a data directory and the filename for the results to evaluate. inputdir is the folder containing original XML (with the ground truth). outputfile is the file name with the entities produced by your system.
- Output: Prints statistics about the predicted entities in the given output file.
- Code:

Note: outputfile must match the pattern: task9.2\_NAME\_NUMBER.txt (where NAME may be any string and NUMBER any natural number). You can use this to encode the program version that produced the file.

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### Detecting interactions - Choosing rules

Function check\_interaction will implement our rule-based interaction detector. Strategy to follow:

- Examine the train data set and try to infer general rules that are right in most cases, even if they seldom apply (high precision, low recall).
  - Look at the text data directly (less useful)
  - Write small scripts that perform some kind of data exploration to find out features that distinguish drug names (more useful)

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### Detecting interactions - Some hints

Example observations that may lead to some rules:

- Pairs with an interaction of type *effect* often have clue words like *administer*, *potentiate*, *prevent*, etc. between e1 and e2.
- Pairs with an interaction of type mechanism often have clue words like reduce, increase, decrease, etc. between e1 and e2.
- Pairs with an interaction of type *int* often have clue words like *interact, interaction,* etc. between e1 and e2.
- Checking for the clue word position (before e1, between e1 and e2, after e2) is a pretty naive heuristics. Better results may be acheved if properties of the dependency tree are used (e.g. e1 is under e2, both e1 and e2 are under the same verb, e1 is [under] the subject of certain verbs (*enhance,reduce,...*), etc.)

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# Outline 1 DDI Baseline General Structure

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### **Evaluating Results**

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Evaluating Results After each change or new rule added, you must check whether it improves the performance of the system. We will evaluate performance using SemEval-2013-Task9 official evaluator. Evaluation goals:

- Find out whether the added rule is useful or damaging
- Find out the weaknesses of our system to decide the target of new rules

### Rule-based Systems Development Methodology

**1** Start with a simple set of rules.

- **2** Use **Train** dataset to get insights about possible rules:
  - Extract statistics or data analysis from Train dataset to find patterns that may be good rules.
  - Run the rules on the **Train** dataset and check system errors and performance statistics to get hints of what needs improvement.
- 3 Create one (or a few) new rules
- 4 Run the new set of rules on the **Devel** dataset. Record the score and save the rules that produced it.
- **5** If the score is better, keep the new rules. If it is worse, back off to best rule set so far. Go to step 2 (or stop when the score is good enough or when no improving rules are found)
- 6 Once a satisfactory set of rules has been established, apply them to **Test** dataset, and record the score.

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### Rule-based Systems Development Methodology

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Evaluating Results • NEVER look at the **Devel** or **Test** dataset.

- Train dataset is used extract information that can be generalized to create new rules.
- Devel dataset is used only to obtain a score and decide whether newly added rules are useful or not.
- Test dataset is used only to obtain a final score on unseen data.

	Exercise Goals
DDI Baseline General Structure Resources Detailed Structure Core task Evaluating Results	Goal 1: Get an overall $F_1$ score of at least 0.15 on <b>Devel</b> dataset.

### Deliverables

Prepare a report containing:

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Evaluating Results For Goal 1:

- Final version of analyze function (and any other subsidiary function used by it).
- Final version of check\_interaction function (and any other subsidiary function used by it).
- Evaluator output for this version on Devel and Test datasets.

All code must be properly commented. Self-contained Jupyter notebooks are acceptable.