Master in Artificial Intelligence

Advanced Human Language Technologies

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FIB

Outline

NERC

the provided baseline recognizes and classifies drug names appearing in the sentences in given file.

```
$ python3 ./baseline-NER.py data/devel.xml index.json
result.out
$ more result.out
DDI-DrugBank.d278.s0|0-9|Enoxaparin|drug
DDI-DrugBank.d278.s0|93-108|pharmacokinetics|group
DDI-DrugBank.d278.s0|113-124|eptifibatide|drug
DDI-MedLine.d88.s0|15-30|chlordiazepoxide|drug
DDI-MedLine.d88.s0|33-43|amphetamine|drug
DDI-MedLine.d88.s0|49-55|cocaine|drug
DDI-MedLine.d88.s1|82-95|benzodiazepine|drug
...
```

The output must be formatted like this, since it is the format expected by the evaluation script.

Data particularities

Examples

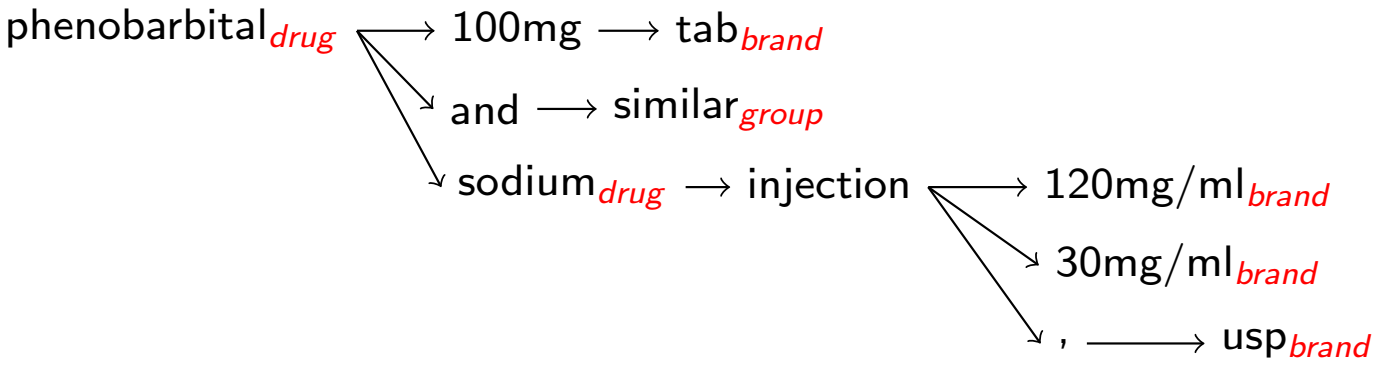
```
<document id="DDI-DrugBank.d284">
    <sentence id="DDI-DrugBank.d284.s0"
            text="If additional adrenergic drugs are to be administered by any route, they should be used with caution because the
                  pharmacologically predictable sympathetic effects of BROVANA may be potentiated.">
        <entity id="DDI-DrugBank.d284.s0.e0" charOffset="14-29" type="group" text="adrenergic drugs"/>
        <entity id="DDI-DrugBank.d284.s0.e1" charOffset="166-172"type="brand" text="BROVANA"/>
        <pair id="DDI-DrugBank.d284.s0.p0" e1="DDI-DrugBank.d284.s0.e0" e2="DDI-DrugBank.d284.s0.e1" ddi="true" type="advise"/>
    </sentence>
    (...)
    <sentence id="DDI-DrugBank.d284.s5"
              text="Although the clinical significance of these effects is not known, caution is advised in the co-administration
                    of beta-agonists with non-potassium sparing diuretics.">
        <entity id="DDI-DrugBank.d284.s5.e0" charOffset="113-125" type="group" text="beta-agonists"/>
        <entity id="DDI-DrugBank.d284.s5.e1" charOffset="132-162" type="group" text="non-potassium sparing diuretics"/>
        <pair id="DDI-DrugBank.d284.s5.p0" e1="DDI-DrugBank.d284.s5.e0" e2="DDI-DrugBank.d284.s5.e1" ddi="true" type="advise"/>
    </sentence>
    (...)
    <sentence id="DDI-DrugBank.d284.s16"
              text="In this setting, cardioselective beta-blockers could be considered, although they should be administered
                    with caution.">
        <entity id="DDI-DrugBank.d284.s16.e0" charOffset="17-45" type="group" text="cardioselective beta-blockers"/>
    </sentence>
</document>
```

Drug names vary in number of words and tokenization elements.

Outline

Simple approach

- Create an index of known groups, and search tokens in input sentence in the index
- To deal with multi-token drug names, the index must be a **prefix tree**
- Tree nodes must correspond to *tokens* according to the same tokenizer used on input data



General structure

The program expects as argument the directory with XML files to process. Results are printed to stdout

```
# Create prefix tree index of known drug names
index = DrugIndex(drugindex)
# create tokenizer
nlp = spacy.load("en_core_web_trf", enable=["tokenizer"])
# parse XML file, obtaining a DOM tree
tree = parse(datafile)
# 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
    print(f"processing sentence {sid}         \r", end="")

    # tokenize text with spacy tokenizer
    tokens = nlp(stext)
    # extract entities in text
    entities = extract_entities(stext, tokens, index)

    # print sentence entities in format requested for evaluation
    for e in entities :
    print(sid,
          e["offset"],
          e["text"],
          e["type"],
          sep = "|",
          file = outf)
```

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Resources

The program uses:

- An XML parser: `xml.dom.minidom` (`https://docs.python.org/3.7/library/xml.dom.minidom.html`, included in python standard libray)
- A tokenizer for English text: `SpaCy` (check `https://spacy.io/usage` if you don't have it installed)
- The evaluator module to compute performance scores (provided in the lab project zipfile).

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Executing the baseline


```
$ python3 run.py
 Extracting drugs from train data
 Creating index with all known drug names
 Collecting drugs from HSDB
 Collecting drugs from DrugBank
 Collecting drugs from drugs-train
 Applying index to predict drugs
 Running baseline on devel
 Evaluating baseline on devel
 Running baseline on test
 Evaluating baseline on test
```

Results

Results on `devel` dataset

	tp	fp	fn	#pred	#exp	P	R	F1
brand	329	165	46	494	375	66.6%	87.7%	75.7%
drug	1800	648	144	2448	1944	73.5%	92.6%	82.0%
drug_n	7	16	93	23	100	30.4%	7.0%	11.4%
group	508	389	198	897	706	56.6%	72.0%	63.4%
M.avg	-	-	-	-	-	56.8%	64.8%	58.1%
m.avg	2644	1218	481	3862	3125	68.5%	84.6%	75.7%
m.avg(no class)	2719	1143	406	3862	3125	70.4%	87.0%	77.8%

Results on `test` dataset

	tp	fp	fn	#pred	#exp	P	R	F1
brand	261	180	14	441	275	59.2%	94.9%	72.9%
drug	1915	582	236	2497	2151	76.7%	89.0%	82.4%
drug_n	8	33	94	41	102	19.5%	7.8%	11.2%
group	534	456	166	990	700	53.9%	76.3%	63.3%
M.avg	-	-	-	-	-	52.3%	67.0%	57.4%
m.avg	2718	1251	510	3969	3228	68.5%	84.2%	75.5%
m.avg(no class)	2872	1097	356	3969	3228	72.4%	89.0%	79.8%

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Conclusions

- A **very** simple approach based on knowledge bases (drug lists) has a pretty good performance (close to 60%macro-average, 80% micro-average).
- If we use machine learning for this task, we should aim to obtain **significantly** better results, or the additional complexity and cost won't pay off.
- Any ML project requires to start with a **baseline** that sets a threshold to calibrate cost/benefit ratio of the project. The baseline should be a simple knowledge-based or basic statistical approach.
- This will be the goal of the first lab task: **Drug NERC**.