

Master in Artificial Intelligence

Advanced Human Language Technologies

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables



UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Facultat d'Informàtica de Barcelona



Outline

1 Machine Learning DDI

2 Relation Extraction

3 General Structure

4 Resources

5 Detailed Structure

- Feature Extractor

- Learner

- Classifier

6 Core task

7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Core task

Goals &
Deliverables

Session 4 - DDI using machine learning

Assignment

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 a **ML classification** algorithm to solve the problem.

```
$ python3 ./ml-DDI.py data/Devel/  
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.d211.s2|DDI-DrugBank.d211.s2.e0|DDI-DrugBank.d211.s2.e5|mechanism  
...
```

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Core task

Goals &
Deliverables

Outline

1 Machine Learning DDI

2 Relation Extraction

3 General Structure

4 Resources

5 Detailed Structure

- Feature Extractor

- Learner

- Classifier

6 Core task

7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Core task

Goals &
Deliverables

Relation Extraction

- Relation Extraction is a NLP task, frequently required in Information Extraction applications.
- The goal of the task is to extract relations between entities (previously detected), expressed in the text. E.g.: `is_CEO_of(Person,Organization)`:
 - *Steve Jobs* was the chairman, the chief executive officer (CEO), and a co-founder of *Apple Inc.*, ...
 - During his career at *Microsoft*, *Bill Gates* held the positions of chairman, chief executive officer (CEO), president and chief software architect.
 - *Mark Zuckerberg* is known for co-founding *Facebook, Inc.* and serves as its chairman, chief executive officer, and controlling shareholder.

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables

Relation Extraction

Other examples:

- **Medical domain:**

- `caused_by(diagnose, drug)`
 - `prescribed_for(drug, diagnose)`
 - `drug_interaction(drug, drug)`

- **Legal domain:**

- `is_suing(Person/Org, Person/Org)`
 - `is_representing(Person, Person/Org)`
 - `is_sentenced_for(Person/Org, Crime)`
 - `is_sentenced_to(Person/Org, Penalty)`

- **Business/Economy:**

- `is_CEO_of(Person, Organization)`
 - `absorbed_by(Organization, Organization)`

- etc.

Relation Extraction

Relation Extraction can be approached as a classical ML classification task, where:

- The objects to be classified are a **text fragment** (sentence, paragraph...) plus a **pair of target entities** in it.
- Each object (*text, entity1, entity2*) is encoded as a feature vector.
- The output class is either **None**, or one **relation type** chosen among a *predefined list*.

Informative enough features are crucial to get good results.

Outline

1 Machine Learning DDI

2 Relation Extraction

3 General Structure

4 Resources

5 Detailed Structure

- Feature Extractor

- Learner

- Classifier

6 Core task

7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

**General
Structure**

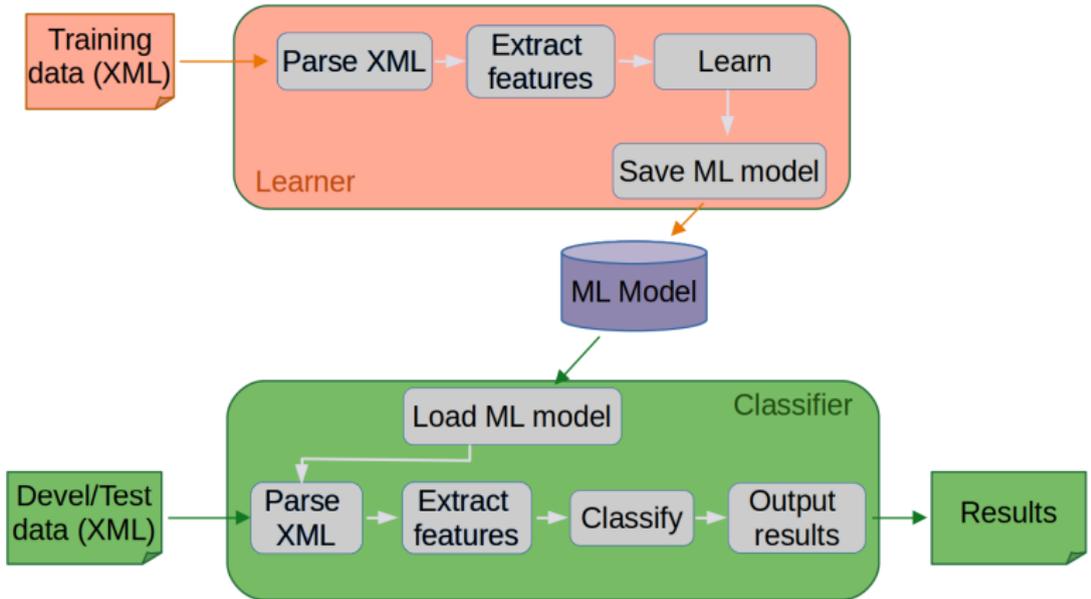
Resources

Detailed
Structure

Core task

Goals &
Deliverables

General Structure



Machine Learning DDI

Relation Extraction

General Structure

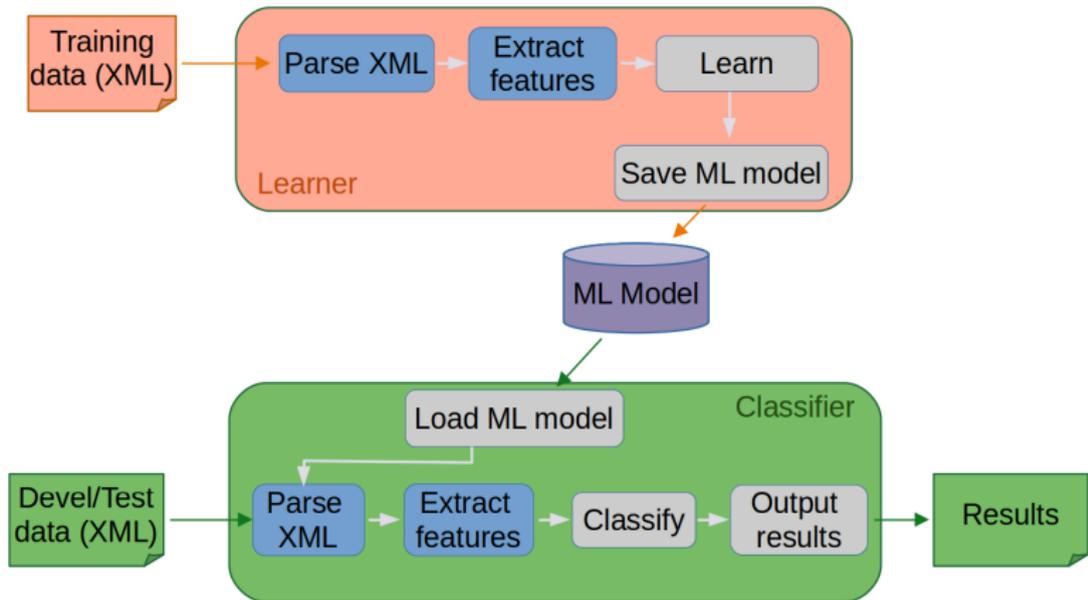
Resources

Detailed Structure

Core task

Goals & Deliverables

General Structure



Extracting features is a costly operation, which we do not want to repeat for every possible experiment or algorithm parametrization.

Machine Learning DDI

Relation Extraction

General Structure

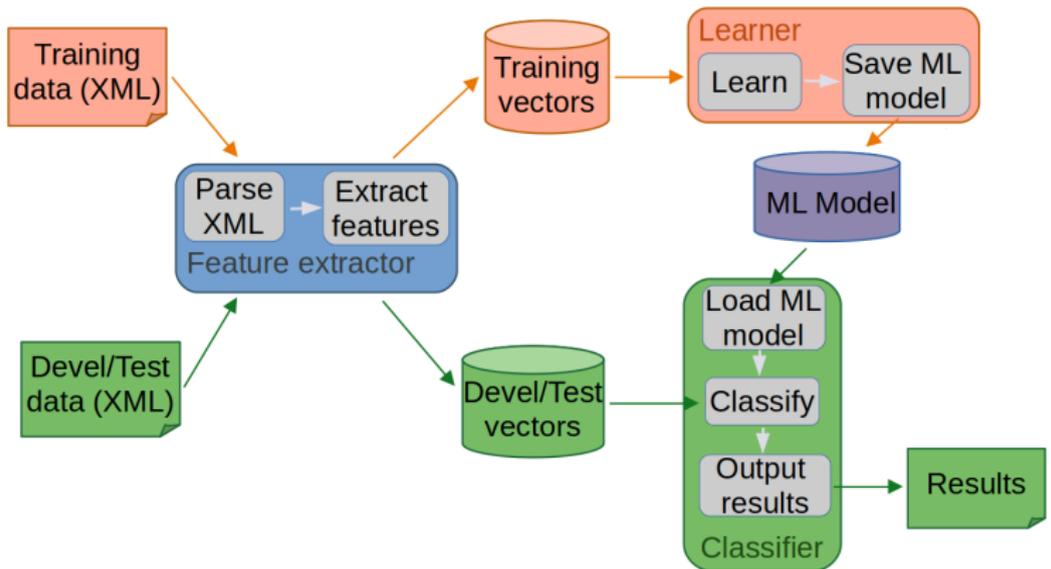
Resources

Detailed Structure

Core task

Goals & Deliverables

General Structure



Feature extraction process is performed once, out of learning or predicting processes.

Machine Learning DDI

Relation Extraction

General Structure

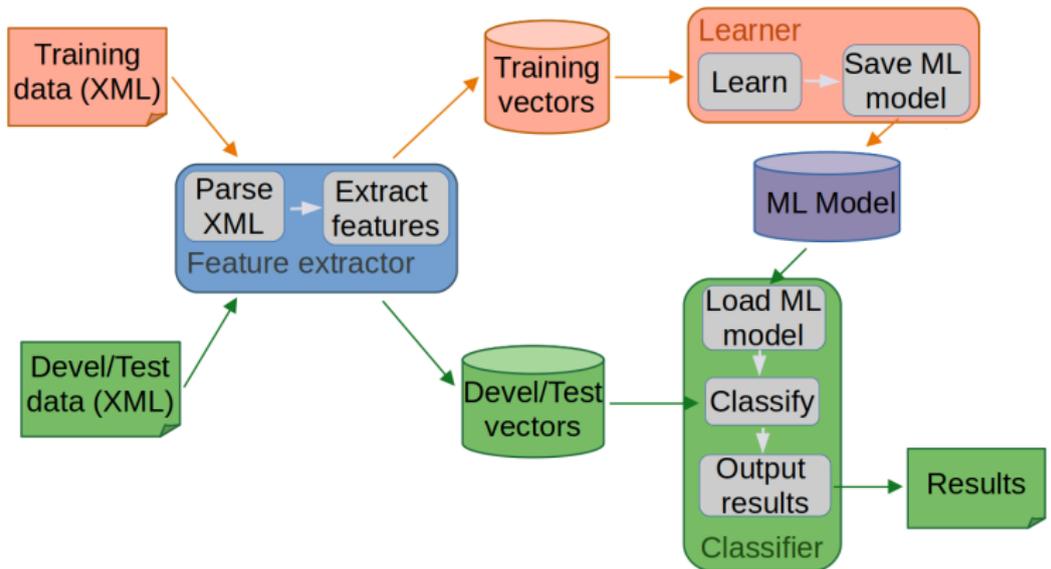
Resources

Detailed Structure

Core task

Goals & Deliverables

General Structure



Feature extraction process is performed once, out of learning or predicting processes.

Thus, we need to write not a single program, but three different components: feature extractor, learner, and classifier.

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables

Outline

1 Machine Learning DDI

2 Relation Extraction

3 General Structure

4 Resources

5 Detailed Structure

- Feature Extractor

- Learner

- Classifier

6 Core task

7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Core task

Goals &
Deliverables

Resources

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

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

Outline

- 1 Machine Learning DDI
- 2 Relation Extraction
- 3 General Structure
- 4 Resources
- 5 Detailed Structure**
 - Feature Extractor
 - Learner
 - Classifier
- 6 Core task
- 7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

**Detailed
Structure**

Core task

Goals &
Deliverables

Outline

- 1 Machine Learning DDI
- 2 Relation Extraction
- 3 General Structure
- 4 Resources
- 5 Detailed Structure**
 - Feature Extractor
 - Learner
 - Classifier
- 6 Core task
- 7 Goals & Deliverables

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Feature Extractor

The feature extractor:

- Independent program, separated from learner and classifier
- Receives as argument the directory with the XML files to encode.
- Prints the feature vectors to stdout

```
$ python3 ./feature-extractor.py data/devel > devel.feats
```

```
$ more devel.feats
```

```
DDI-DrugBank.d339.s0 DDI-DrugBank.d339.s0.e0 DDI-DrugBank.d339.s0.e1 null lib=elevated  
wib=Elevated lpib=elevated_JJ la2=level wa2=levels lpa2=level.NNS la2=have wa2=have  
lpa2=have_VBP la2=be wa2=been lpa2=be_VBN la2=report (...) lpa2=concomitantly_RB path1=NNP  
path2=NNP\dep\nsubjpass\compound path=NNP\dep\nsubjpass\compound  
DDI-DrugBank.d339.s0 DDI-DrugBank.d339.s0.e0 DDI-DrugBank.d339.s0.e2 null lib=elevated  
wib=Elevated lpib=elevated_JJ wib=experience lpib=experience_NN la2=be wa2=is lpa2=be_VBZ  
la2=administer wa2=administered lpa2=administer_VBN la2=concomitantly wa2=concomitantly  
lpa2=concomitantly_RB path1=NNP path2=NNP\dep\advcl\advcl\nsubjpass  
path=NNP\dep\advcl\advcl\nsubjpass  
DDI-DrugBank.d339.s0 DDI-DrugBank.d339.s0.e1 DDI-DrugBank.d339.s0.e2 mechanism  
lb1=carbamazepine wb1=Carbamazepine wb1=Elevated lpb1=elevated_JJ lib=level wib=levels  
lpib=level.NNS lib=have wib=have lpib=have_VBP lib=be wib=been lpib=be_VBN lib=report  
wib=reported lpib=report_VBN lib=postmarket wib=postmarketing lpib=postmarket_VBG  
lib=experience wib=experience lpib=experience_NN la2=be wa2=is lpa2=concomitantly_RB  
path1=compound/nsubjpass/VBN path2=VBN\advcl\advcl\nsubjpass  
path=compound/nsubjpass/VBN\advcl\advcl\nsubjpass  
...
```

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Feature Extractor

```
# 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 ground truth entities
        entities = {}
        ents = s.getElementsByTagName("entity")
        for e in ents :
            id = e.attributes["id"].value
            entities[id] = e.attributes["charOffset"].value.split("-")
        # analyze sentence if there is at least a pair of entities
        if len(entities) <= 1: continue

    analysis = deptree(stext)
    # for each pair of entities, decide whether it is DDI and its type
    pairs = s.getElementsByTagName("pair")
    for p in pairs:
        # get ground truth
        ddi = p.attributes["ddi"].value
        dditype = p.attributes["type"].value if ddi=="true" else "null"
        # target entities
        id_e1 = p.attributes["e1"].value
        id_e2 = p.attributes["e2"].value
        # feature extraction
        feats = extract_features(analysis, entities, id_e1, id_e2)
        # resulting feature vector
        print(sid, id_e1, id_e2, dditype, "\t".join(feats), sep="\t")
```

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Feature Extractor

Core task

Goals &
Deliverables

Feature Extractor Functions - Extract features

```
def extract_features(tree, entities, e1, e2) :  
    '''  
    Task:  
        Given an analyzed sentence and two target entities, compute a feature  
        vector for this classification example.  
  
    Input:  
        tree: 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 for an interaction  
  
    Output:  
        A vector of binary features.  
        Features are binary and vectors are in sparse representation (i.e. only  
        active features are listed)  
  
    Example:  
  
    >>> extract_features(tree, {'DDI-DrugBank.d370.s1.e0':['43','52'],  
                               'DDI-DrugBank.d370.s1.e1':['57','70'],  
                               'DDI-DrugBank.d370.s1.e2':['77','88']},  
                          'DDI-DrugBank.d370.s1.e0', 'DDI-DrugBank.d370.s1.e2')  
    ['lbi=Caution', 'lbi=be', 'lbi=exercise', 'lbi=combine', 'lib=or', 'lib  
    =salicylic', 'lib=acid', 'lib=with', 'LCSpos=VBG', 'LCSlema=combine',  
    'path=dobj/combine\nmod\compound' 'entity_in_between']  
    ,,,
```

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Feature Extractor

Core task

Goals &
Deliverables

Feature Extractor - Relevant Features

- Presence of certain *clue verbs* may be indicative of the interaction type.
- Clue verb position (before/inbetween/after) with respect to the target entities.
- Presence of other entities in between.
- Words, lemmas, PoS (or combinations of them) appearing before/inbetween/after the target pair.

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Feature Extractor - Relevant Features

- Presence of certain *clue verbs* may be indicative of the interaction type.
- Clue verb position (before/inbetween/after) with respect to the target entities.
- Presence of other entities in between.
- Words, lemmas, PoS (or combinations of them) appearing before/inbetween/after the target pair.
- **Features encoding information from the syntactic tree.**

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

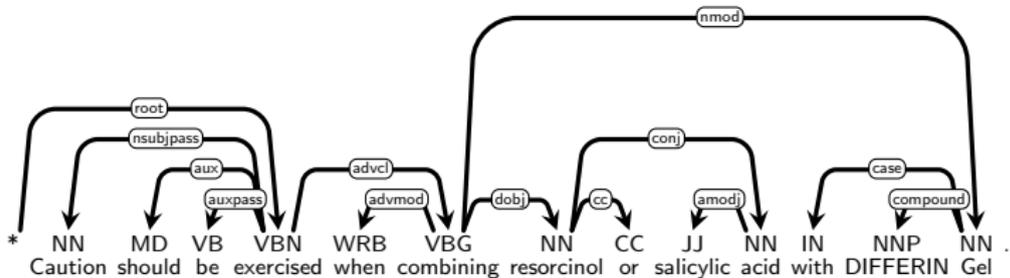
Goals & Deliverables

Feature Extractor - Relevant Features

- Presence of certain *clue verbs* may be indicative of the interaction type.
- Clue verb position (before/inbetween/after) with respect to the target entities.
- Presence of other entities in between.
- Words, lemmas, PoS (or combinations of them) appearing before/inbetween/after the target pair.
- **Features encoding information from the syntactic tree.**

Remember: All features are *binary features* (they are either present or not present in a given example) and examples are encoded as *sparse vectors* (lists feature names present in the example)

Feature Extractor - Path Features



Entities:

e0: resorcinol

e1: salicylic acid

e2: DIFFERIN Gel

Example path features:

PAIR (e0,e1)

Tree fragment: $e0 \xrightarrow{conj} e1$

(e1 is direct child of e0. The arc is labeled *conj*)

Feature name: **path=conj**>

Machine Learning DDI

Relation Extraction

General Structure

Resources

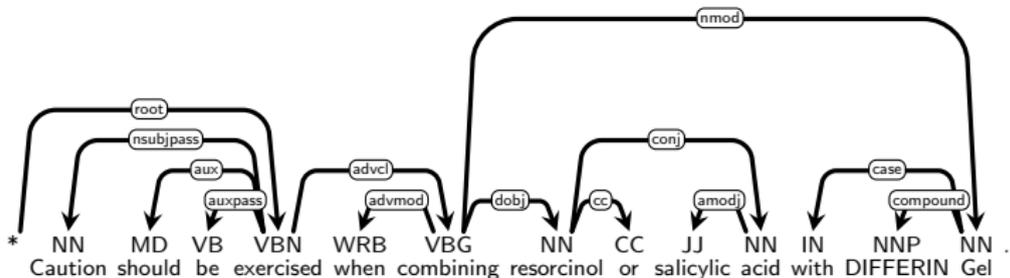
Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Feature Extractor - Path Features



Entities:

e0: resorcinol

e1: salicylic acid

e2: DIFFERIN Gel

Example path features:

PAIR (e0,e2)

Tree fragment: e0 \xleftarrow{dobj} combine \xrightarrow{nmod} e2

(e0 is direct child of verb "combine" with label *dobj*, and e2 is direct child of the same verb, with label *nmod*)

Feature name: path=dojb<combine>nmod

Machine Learning DDI

Relation Extraction

General Structure

Resources

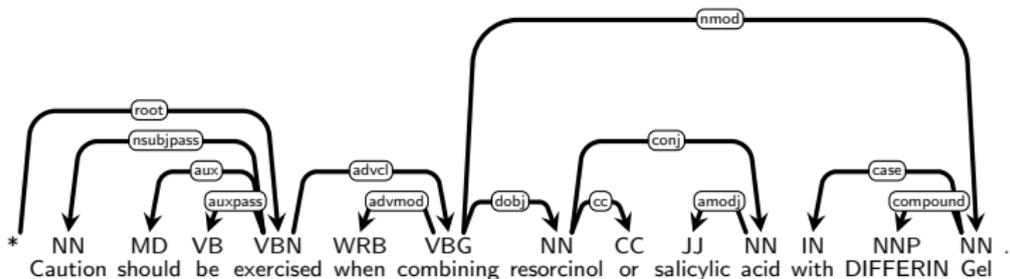
Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Feature Extractor - Path Features



Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Entities:

e0: resorcinol

e1: salicylic acid

e2: DIFFERIN Gel

Example path features:

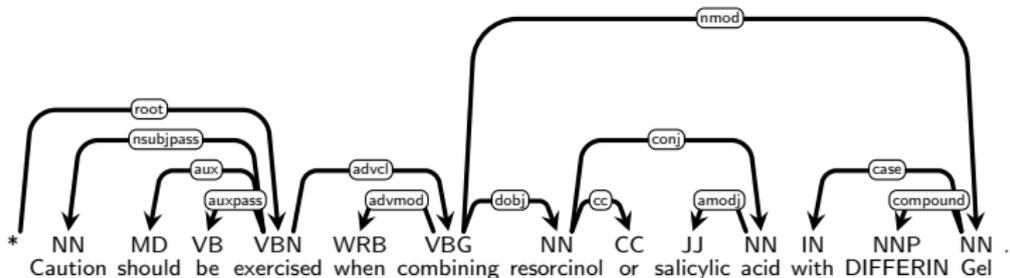
PAIR (e1,e2)

Tree fragment: e1 \xleftarrow{conj} resorcinol \xleftarrow{dobj} combine \xrightarrow{nmod} e2

(e1 is *conj* child of "resorcinol", which is under verb "combine" with label *dobj*, and e2 is direct child of the same verb, with label *nmod*)

Feature name: **path=conj<dobj<combine>nmod**

Feature Extractor - Path Features



Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Entities:

e0: resorcinol

e1: salicylic acid

e2: DIFFERIN Gel

Example path features:

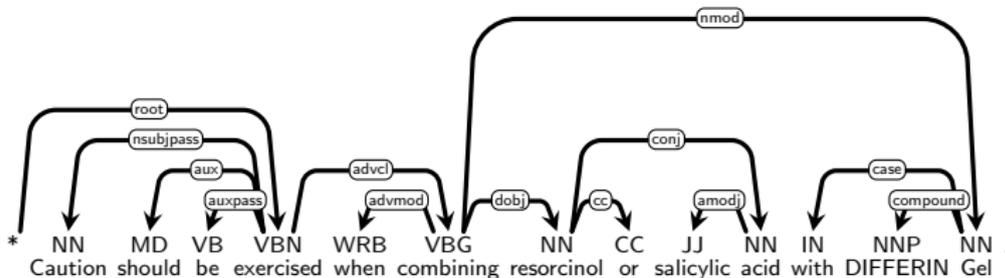
PAIR (e1,e2)

Tree fragment: $e1 \xleftarrow{conj} \text{resorcinol} \xleftarrow{dobj} \text{combine} \xrightarrow{nmod} e2$

(e1 is *conj* child of "resorcinol", which is under verb "combine" with label *dobj*, and e2 is direct child of the same verb, with label *nmod*)

Also possible: **path=conj<ENTITY/dobj<combine>nmod**

Feature Extractor - Path Features



Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Feature Extractor

Core task

Goals & Deliverables

Entities:

e0: resorcinol

e1: salicylic acid

e2: DIFFERIN Gel

Example path features:

PAIR (e1,e2)

Tree fragment: $e1 \xleftarrow{conj} \text{resorcinol} \xleftarrow{doobj} \text{combine} \xrightarrow{nmod} e2$

(e1 is *conj* child of "resorcinol", which is under verb "combine" with label *doobj*, and e2 is direct child of the same verb, with label *nmod*)

Also possible: `path=doobj*<combine>nmod`

Feature Extractor - Path Features

Path features may be build in different ways, encoding different information about the tree

- Node words
- Node lemmas
- Node PoS
- Edge labels
- Edge direction
- Direct/indirect dependencies
- ... or any combination of these ...

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Feature Extractor

Core task

Goals &
Deliverables

Feature Extractor - Path Features

Path features may be build in different ways, encoding different information about the tree

- Node words
- Node lemmas
- Node PoS
- Edge labels
- Edge direction
- Direct/indirect dependencies
- ... or any combination of these ...

Remember: All features are *binary features* (they are either present or not present in a given example) and examples are encoded as *sparse vectors* (lists of present feature names)

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Feature Extractor

Core task

Goals &
Deliverables

Outline

- 1 Machine Learning DDI
- 2 Relation Extraction
- 3 General Structure
- 4 Resources
- 5 Detailed Structure**
 - Feature Extractor
 - Learner**
 - Classifier
- 6 Core task
- 7 Goals & Deliverables

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Learner

Core task

Goals & Deliverables

Learner - Option 1: Maximum Entropy

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Learner

Core task

Goals & Deliverables

- Use `megam` to train a model as seen in class
- `megam` does not expect the extra information in the features file, thus the first 3 fields (`sent_id`, `ent_id1`, `ent_id`) must be removed:

```
python3 extract-features.py data/train | cut -f4- > train.feats
./megam-64.opt -nc -nobias multiclass train.feats >model.MEM
```

Learner - Option 2: Your choice

- Select a ML algorithm of your choice (DT, SVM, RF, ...) and a python library implementing it.
- Adapt the feature file format to the needs of the selected algorithm
- Train a classification model for the task of **classifying** entity pairs.

Note that the target task is a mere classification, not a sequence prediction. So, for a given sentence and pair of entities in it, the output is just **one** label, not a sequence. Thus, sequence labeling algorithms such as CRFs are overdimensioned (and probably not straightforward to apply).

Outline

- 1 Machine Learning DDI
- 2 Relation Extraction
- 3 General Structure
- 4 Resources
- 5 Detailed Structure**
 - Feature Extractor
 - Learner
 - Classifier**
- 6 Core task
- 7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Classifier

Core task

Goals &
Deliverables

Classifier

```
# read each vector in input file
for line in sys.stdin:
    # split line into elements
    fields = line.strip('\n').split("\t")
    # first 4 elements are sid,e1,e2, and ground
    # truth (ignored since we are classifying)
    (sid,e1,e2,gt) = fields[0:4]

    # Rest of elements are features, passed to the
    # classifier of choice to get a prediction
    prediction = mymodel.classify(fields[4:])

    # if the classifier predicted a DDI, output it
    # in the right format
    if prediction != "null" :
        print(sid,e1,e2,prediction,sep="|")
```

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Classifier

Core task

Goals &
Deliverables

Outline

- 1 Machine Learning DDI
- 2 Relation Extraction
- 3 General Structure
- 4 Resources
- 5 Detailed Structure
 - Feature Extractor
 - Learner
 - Classifier
- 6 Core task**
- 7 Goals & Deliverables

Machine Learning DDI

Relation Extraction

General Structure

Resources

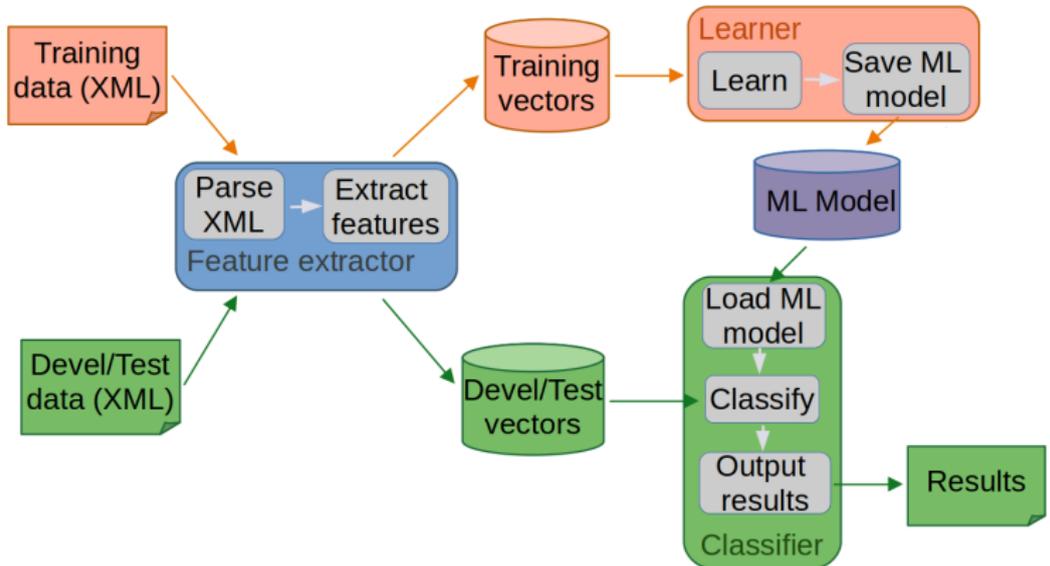
Detailed Structure

Core task

Goals & Deliverables

Build a good ML-based DDI detector

Strategy to follow:



Machine Learning DDI

Relation Extraction

General Structure

Resources

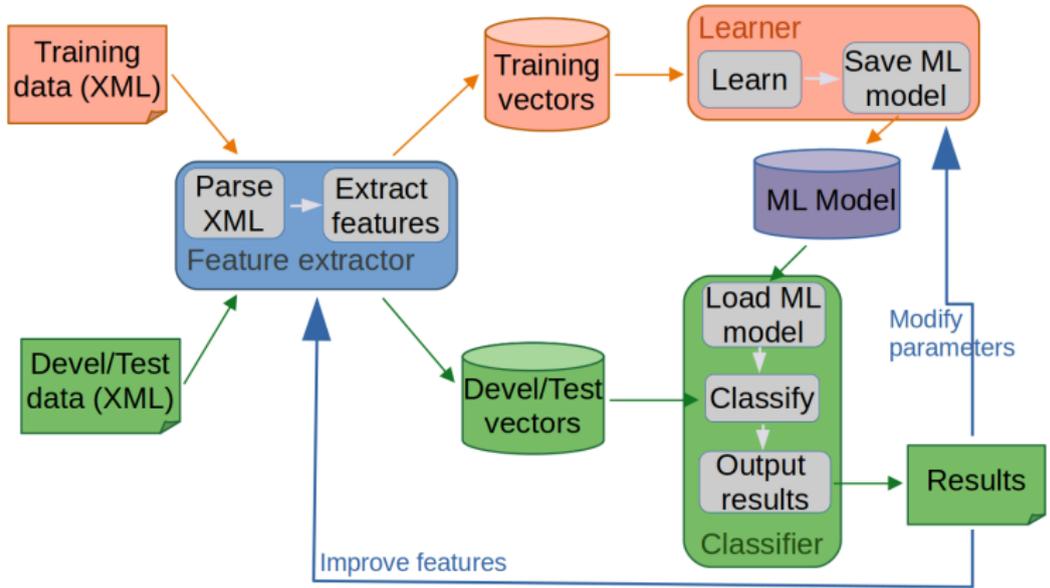
Detailed Structure

Core task

Goals & Deliverables

Build a good ML-based DDI detector

Strategy to follow:



Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables

Detecting interactions: Possible features

Some feature possibilities to explore:

- Features detailing the position of words in the sentence (e.g. before E1, between E1 and E2, after E2)
- More general (or more specific) path features (with/without all elements in the path, lemma/tag of each, etc)
- Features encoding specific tree patterns (and maybe their combination with certain verbs). E.g. Features stating whether patterns used in Task 3 apply.
- Information about the LCS (PoS, lemma, ...)
- Features considering lists of relevant verbs.
- Type of entities in the pair
- Presence of a third entity (in the sentence, in between the target pair, in the path connecting the pair in the tree, ...)
- ...

Outline

- 1 Machine Learning DDI
- 2 Relation Extraction
- 3 General Structure
- 4 Resources
- 5 Detailed Structure
 - Feature Extractor
 - Learner
 - Classifier
- 6 Core task
- 7 Goals & Deliverables

Machine
Learning DDI

Relation
Extraction

General
Structure

Resources

Detailed
Structure

Core task

Goals &
Deliverables

Exercise Goals

What you should do:

- Work on your feature extractor. It is the component of the process where you have most control.
- Pay special attention to features encoding **syntactic information**.
- Experiment with different parameterizations of the chosen learner. You may try different learning algorithms if you feel up to. Note that the same feature vectors can be fed to different learners.
- Keep track of tried features and parameter combinations.

What you should **NOT** do:

- Use neural network learners. We'll do that later on the course.
- Alter the suggested code structure.
- Produce an overfitted model: If performance on the test dataset is much lower than on devel dataset, you probably are overfitting your model.

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables

Exercise Goals

Orientative results

- Provided feature extractor uses 7 feature templates and gets a macroaverage F1 about 50%. Used information includes :
 - word forms, lemmas, and PoS tags (and combinations) appearing in between the target pair.
 - information on the path connecting both target entities: whole path, path from e1 to LCS, path from e2 to LCS.
 - information on the LCS lemma if one entity is under its subject and the other under its object.
- Extending feature repertoire with different pieces of information from the tree, and experimenting with learner parameters should raise macroaverage F1 on devel up to ~60%.

Deliverables

Write a report describing the work carried out in this exercise.

The report must be a **single self-contained PDF document**, under ~10 pages, containing:

- *Introduction*: What is this report about. What is the goal of the presented work.
- *Rule-based baseline*
 - *Ruleset construction*: What did you observe in the data exploration. Which rules did you write according to those observations.
 - *Code*: Include your `check_interaction` function (and **any other function** it may call), properly formatted and commented. **Do not include any other code.**
 - *Experiments and results*: Results obtained on the **devel** and **test** datasets, for different rule combinations you deem relevant.

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables

Deliverables (continued)

- *Machine learning DDI*

- *Selected algorithm*: Which classifier/s did you select or try. Reasons of the choice. Comparison if you tried more than one.
 - *Feature extraction*: Tried/discarded/used features. Impact of different feature combinations
 - *Code*: Include your `extract_features` function (and **any other function** it may call), properly formatted and commented. **Do not include any other code.**
 - *Experiments and results*: Results obtained on the **devel** and **test** datasets, for different algorithms, feature combinations, parameterizations you deem relevant.
- *Conclusions*: Final remarks and insights gained in this task.

Keep result tables in your report in the format produced by the evaluator module. Do not reorganize/summarize/reformat the tables or their content.

Machine Learning DDI

Relation Extraction

General Structure

Resources

Detailed Structure

Core task

Goals & Deliverables