

# RecSys.Scifi: RECOMMENDER SYSTEMS DATASETS IN SCIENTIFIC FIELDS

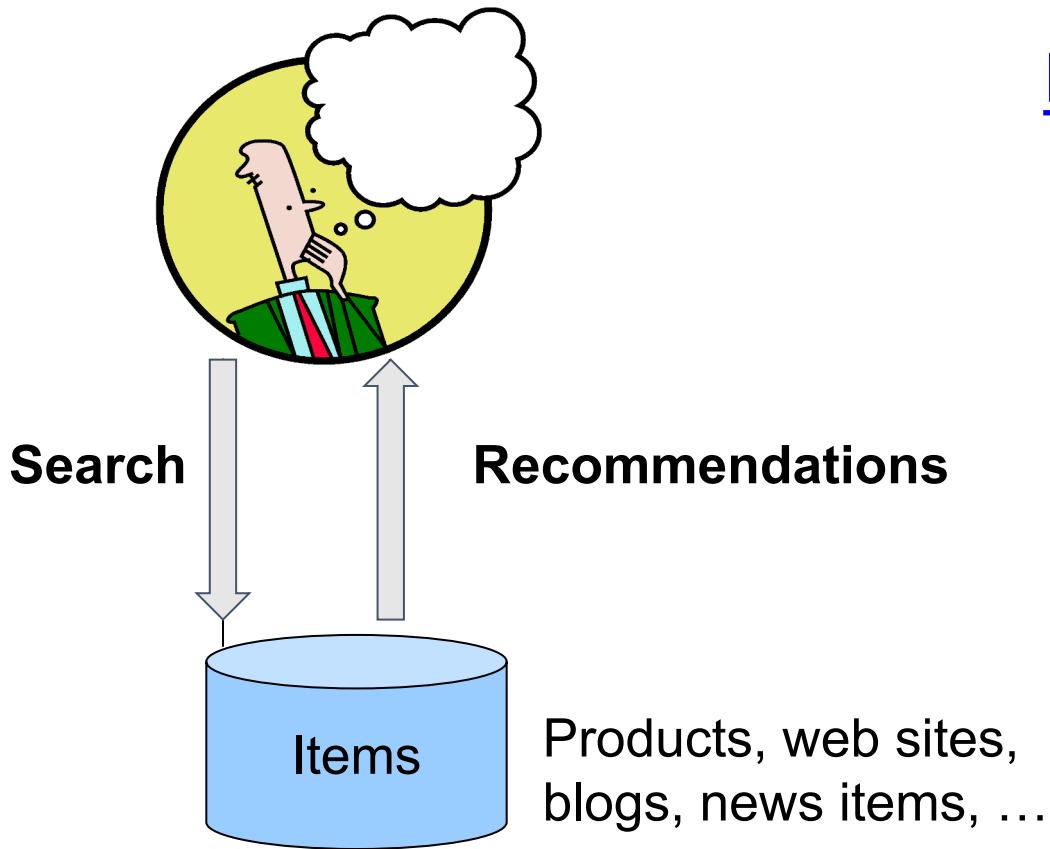
KDD2021 Lecture-style Tutorial

# PART 1

# Introduction to Recommender Systems

**Francisco M. Couto**

# Recommendations



## Examples:

amazon.com.



StumbleUpon



del.icio.us



movieLens  
helping you find the *right* movies

last.fm™  
the social music revolution

Google™  
News

YouTube

XBOX  
LIVE

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

# Long Tail



Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

## Editorial and hand curated

- List of favorites
- Lists of “essential” items

## Simple aggregates

- Top 10, Most Popular, Recent Uploads

## Tailored to individual users

- Amazon, Netflix, ...

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

$X$  = set of **Customers**

$S$  = set of **Items**

**Utility function**  $u: X \times S \rightarrow R$

- $R$  = set of ratings
- $R$  is a totally ordered set
- e.g., 0-5 stars, real number in  $[0,1]$

# Utility Matrix

	Avatar	LOTR	Matrix	Pirates
Alice	1		0.2	
Bob		0.5		0.3
Carol	0.2		1	
David				0.4

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

## (1) Gathering “known” ratings for matrix

- How to collect the data in the utility matrix

## (2) Extrapolate unknown ratings from the known ones

- Mainly interested in high unknown ratings
  - We are not interested in knowing what you don't like but what you like

## (3) Evaluating extrapolation methods

- How to measure success/performance of recommendation methods

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

## Explicit

- Ask people to rate items
- Doesn't work well in practice – people can't be bothered

## Implicit

- Learn ratings from user actions
  - E.g., purchase implies high rating
- What about low ratings?

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

**Key problem:** Utility matrix  $U$  is **sparse**

- Most people have not rated most items
- **Cold start:**
  - New items have no ratings
  - New users have no history

**Three approaches to recommender systems:**

- **1)** Content-based
- **2)** Collaborative
- **3)** Hybrid

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

**Main idea:** Recommend items to customer  $x$  similar to previous items rated highly by  $x$

*Example:*

## Movie recommendations

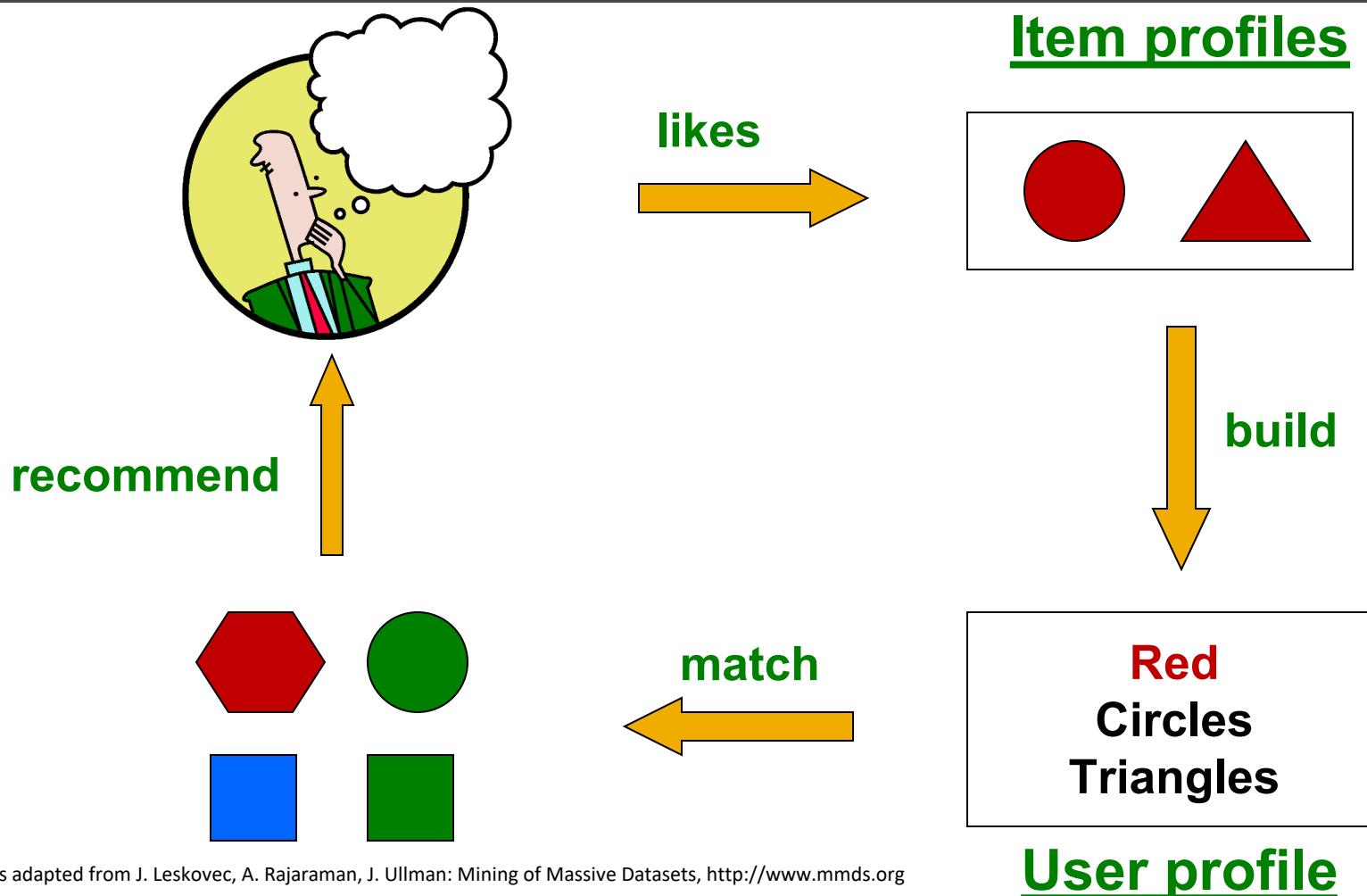
- Recommend movies with same actor(s), director, genre, ...

## Websites, blogs, news

- Recommend other sites with “similar” content

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

# Plan of Action



Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

For each item, create an **item profile**

**Profile is a set (vector) of features**

- **Movies:** author, title, actor, director,...
- **Text:** Set of “important” words in document

**How to pick important features?**

- Usual heuristic from text mining is **TF-IDF**  
(Term frequency \* Inverse Doc Frequency)
  - **Term ... Feature**
  - **Document ... Item**

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

- **User profile possibilities:**

- Weighted average of rated item profiles
- **Variation:** weight by difference from average rating for item
- ...

- **Prediction heuristic:**

- Given user profile  $x$  and item profile  $i$ , estimate

$$u(x, i) = \cos(x, i) = \frac{x \cdot i}{\|x\| \cdot \|i\|}$$

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

**+: No need for data on other users**

- No cold-start or sparsity problems

**+: Able to recommend to users with unique tastes**

**+: Able to recommend new & unpopular items**

- No first-rater problem

**+: Able to provide explanations**

- Can provide explanations of recommended items by listing content-features that caused an item to be recommended

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

- : Finding the appropriate features is hard**
  - E.g., images, movies, music
- : Recommendations for new users**
  - **How to build a user profile?**
- : Overspecialization**
  - Never recommends items outside user's content profile
  - People might have multiple interests
  - Unable to exploit quality judgments of other users**

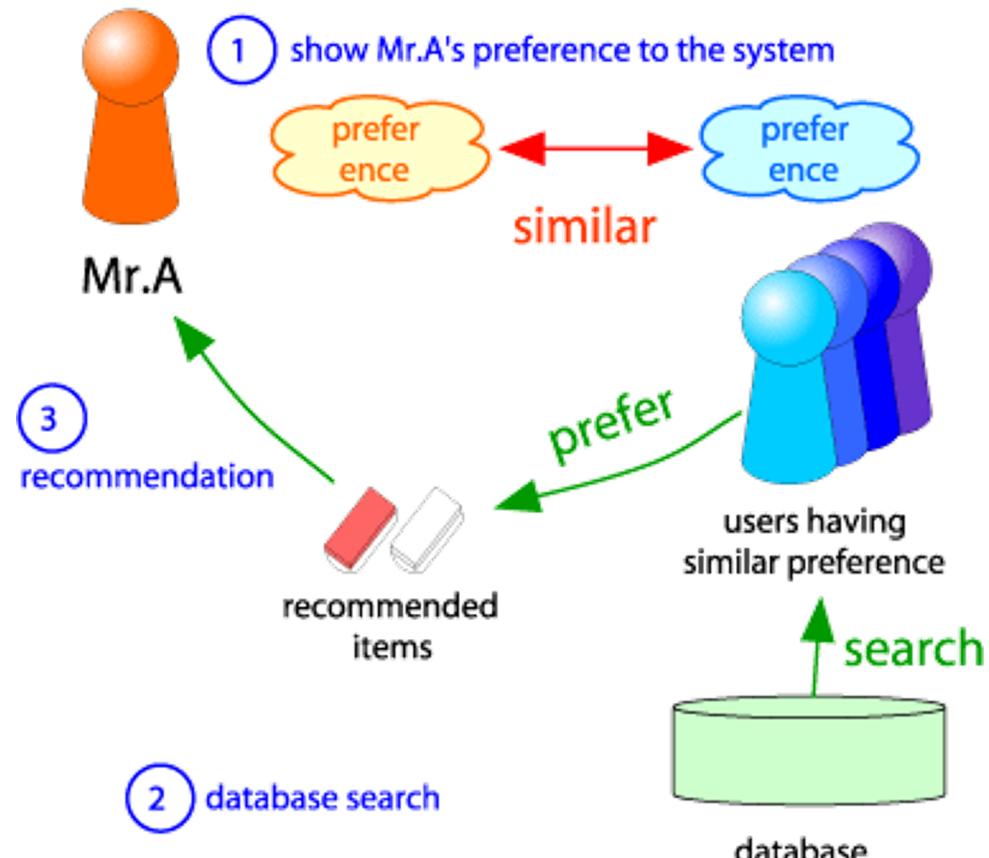
Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

# Collaborative Filtering

Consider user  $x$

Find set  $N$  of other users whose ratings are “similar” to  $x$ 's ratings

Estimate  $x$ 's ratings based on ratings of users in  $N$



Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

## + Works for any kind of item

- No feature selection needed

## - Cold Start:

- Need enough users in the system to find a match

## - Sparsity:

- The user/ratings matrix is sparse
- Hard to find users that have rated the same items

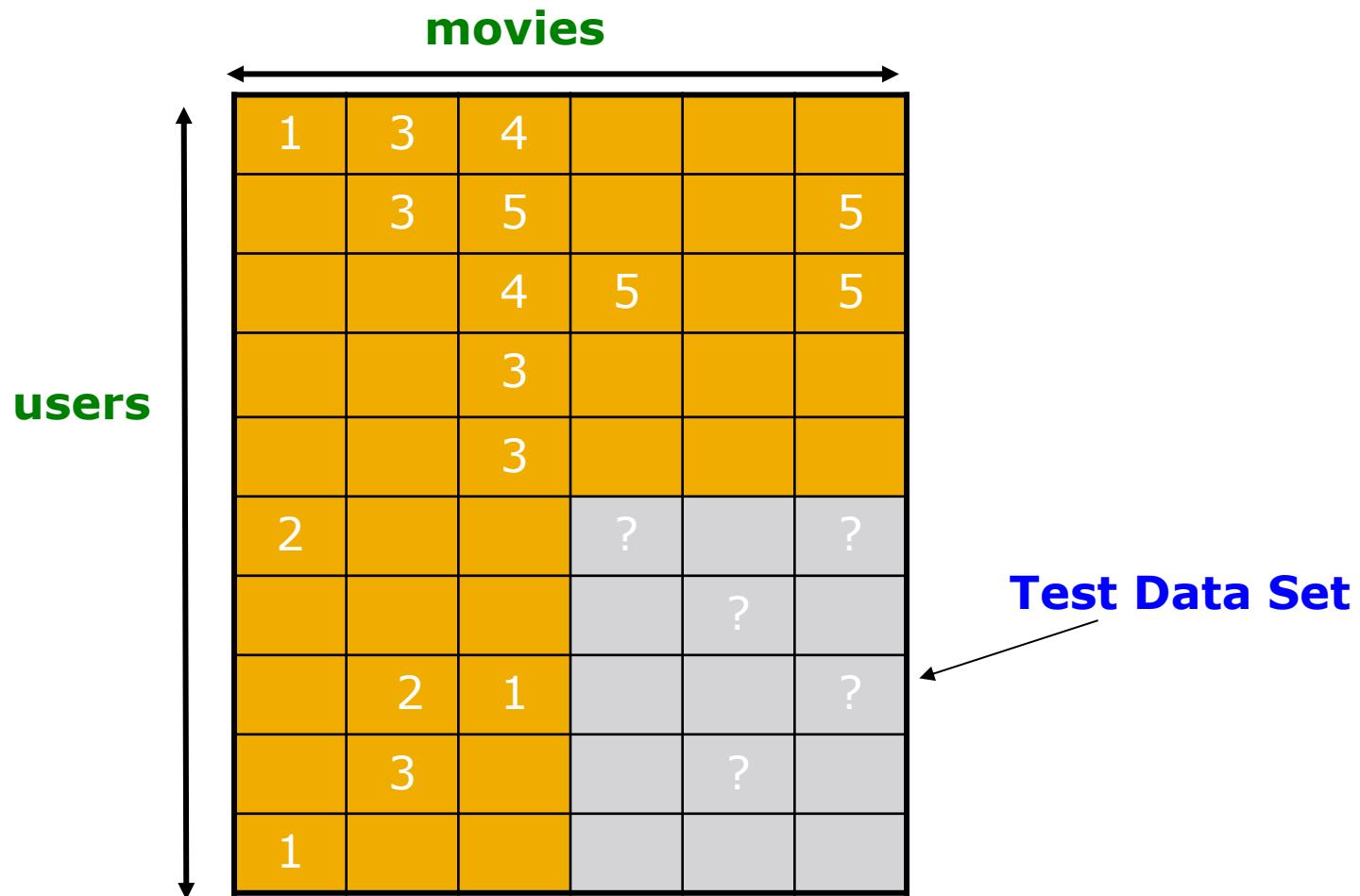
## - First rater:

- Cannot recommend an item that has not been previously rated
- New items, Esoteric items

## - Popularity bias:

- Cannot recommend items to someone with unique taste
- Tends to recommend popular items

# Offline Evaluation



Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

## Predict the rating a user would give to an item

- Root-mean-square error (RMSE)
  - differences between the real and predicted ratings for all items
- Rank Correlation:
  - Spearman's correlation between system and user complete rankings

## Recommend a ranked list of (top@k) items

- Precision@k , Recall@k and F\_measure@k
- Mean Reciprocal Rank (MRR)
- Normalized Discounted Cumulative Gain (nDGC)

Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, <http://www.mmds.org>

## A/B testing

- Test different algorithms on-the-fly
- Measure #Recommendations followed
- Pros: measure real impact on users
- Cons: only available to data platform owners

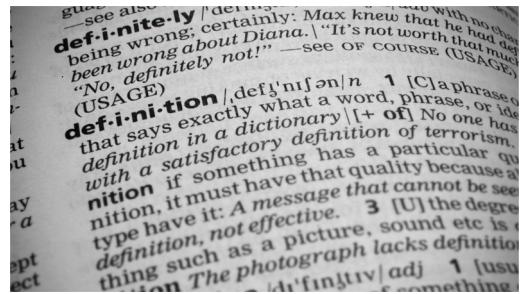
# Scientific recommender systems

**Matilde Pato**

# Scientific fields

Concepts and definitions

What is mean **Scientific Fields?**



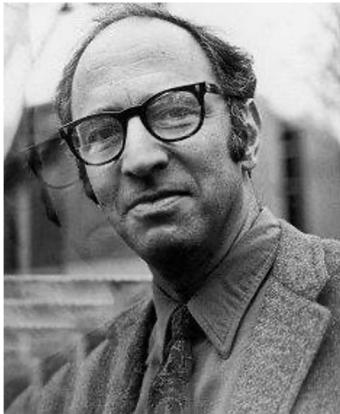
“particular branches of study or spheres of activity or interest”

Oxford Dictionaries. 2021.

# Scientific fields

Concepts and definitions

What is mean **Scientific Fields**?



Thomas S. Kuhn (1922-1996)

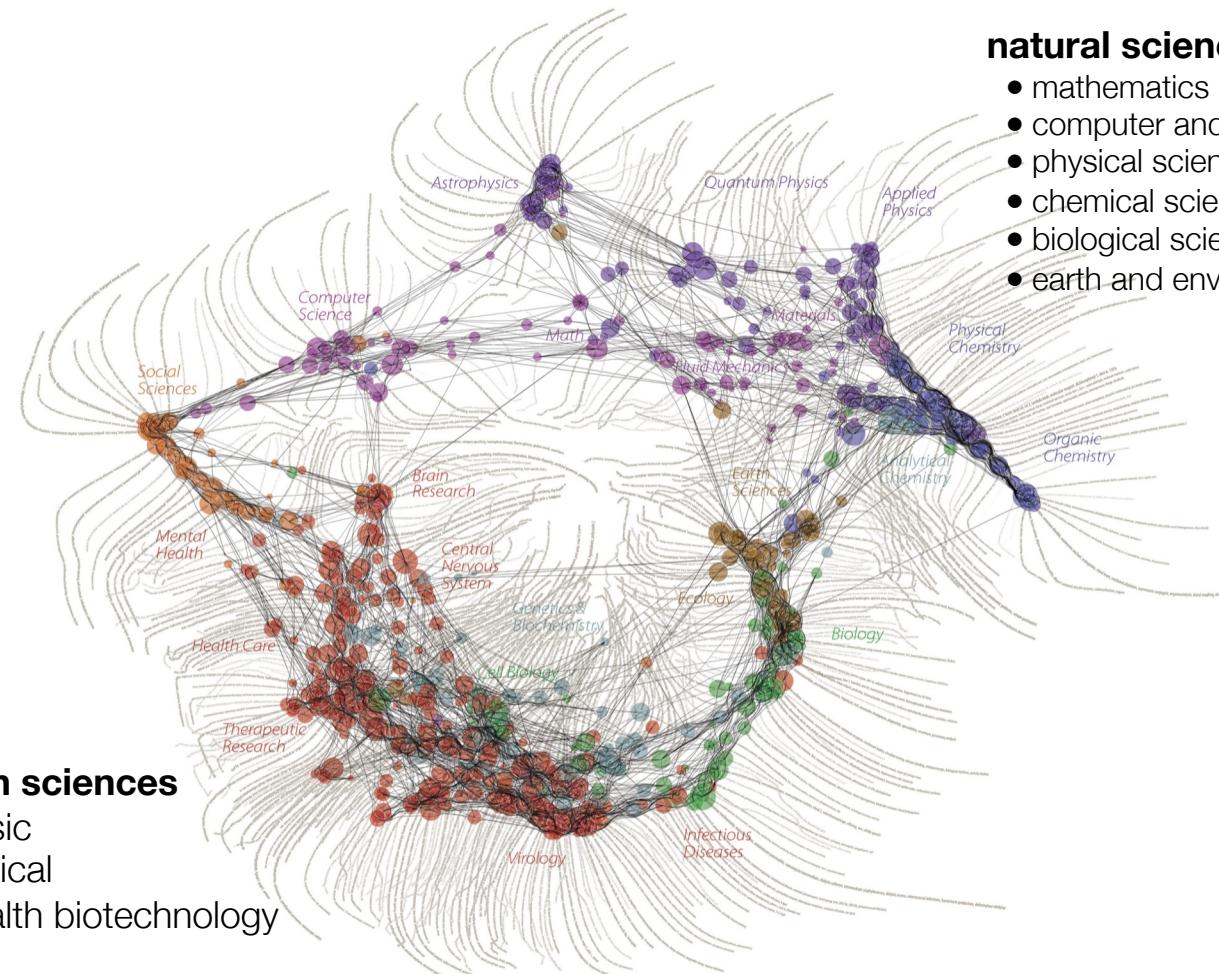
*“Acquisition of a paradigm and of the more esoteric type of research it permits a sign of maturity in the development of any given scientific field”* (Structure of Scientific Revolutions, 1970)

Years after the publication of “The Structure of Scientific Revolutions”, Kuhn dropped the concept of a paradigm and began to focus on the semantic aspects of scientific theories ... (The Road since Structure, 2000)

# Scientific fields

Branches of science

## social sciences



## health sciences

- basic
- clinical
- health biotechnology

Research & Node Layout: Kevin Boyack and Dick Klavans (mapofscience.com); Data: Thompson ISI; Graphics & Typography: W. Bradford Paley (didi.com/brad); Commissioned Katy Börner (scimaps.org)

# Scientific items

## Concepts and definitions



### What is mean **Scientific Items**?

IEEE Access

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#### Using Research Literature to Generate Datasets of Implicit Feedback for Recommending Scientific Items

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**ABSTRACT** In an age of information overload, we are faced with seemingly endless options from which to choose what we want to make for consumption, what we search, require and value more. Recommender Systems have long become the key tool for assisting users in their choices. Interestingly, the use of Recommender Systems for recommending scientific items remains a rarity. One difficulty for this is the lack of datasets available with the ratings of the users for books, music, or films. While there are several datasets available with the ratings of the users for books, music, or films, there is a lack of similar datasets for scientific fields, such as Astronomy and Life and Health Sciences. To address this, this paper proposes a methodology for generating datasets of implicit feedback for recommending scientific items. The proposed methodology consists in identifying a list of items, finding research articles related to these items, and then extracting the names of the authors who wrote these articles. The unique authors from the collected articles, and the rating values are the number of articles a unique author wrote about an item. Considering that literature is available for every scientific field, the methodology is applied to two distinct scientific fields: Life and Health Sciences and Astronomy. The generated dataset, LIBRETTI (LITERature Based REcommendaTion of scientific Items), was assessed in two study cases, Astronomy and Chemistry. Several evaluation metrics for the datasets generated with LIBRETTI were computed, and the results show that the generated datasets are suitable for the use of recommender algorithms. The results were found to be similar, which provides a solid indication that LIBRETTI is a promising approach for generating datasets of implicit feedback for recommending scientific items.

**INDEX TERMS** Recommender systems, collaborative filtering, scientific literature dataset, astronomy, chemical compounds.

#### I. INTRODUCTION

In the last years, scientific literature has increased in size and complexity [1]. Scientific literature has several applications and purposes, but the main goal is to disseminate the work done by researchers. Recommender Systems (RSs) and RSs have been a useful help to that end, by improving the discoverability of research articles.

Recently, there has been a proposal of a methodology for generating datasets of implicit feedback, suitable for evaluating recommender algorithms in scientific areas, by going beyond

the recommendation of books, and articles, and support the recommendation of scientific items. For the purpose of this work, we define scientific items as an entity belonging to the universe, that may be modeled, characterized by multiple features, and used as an object of study in a particular area of research. Some examples of scientific items are genes, phenotypes, chemical entities, plants, diseases, stars, and groups of galaxies.

RSs are software tools that provide suggestions for items that are presumably of interest to a particular user [2], which can be used in a variety of domains, such as a wide range of products, for example, movies, books, research articles, or e-commerce [3]–[5]. Some well-known platforms integrating

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“(...) an entity belonging to universe, that may be modeled, characterized by multiple features using computational representation, and an object of research.”

Barros et al in IEEE Access 2019, 7, pp. 176668-176680

“(...) genes, phenotypes, **chemical entities**, plants, **disease**, stars”

# Literature review

## Search process

### 4 databases

1. ACM Digital Library
2. IEEE Computer Science
3. Elsevier
4. Springer Link

### 2 search engines

1. Google Scholar
2. Semantic Scholar

### search algorithm

- { {recommender OR recommendation} AND {system OR engine} AND ... }
1. {drug OR medication} }
  2. {chemical compounds OR drug} }
  3. {disease} }
  4. include “AND {dataset}”

# Literature review

Search process

## include

1. conference proceeding and journal published after 2009 to present
2. studies focusing on *scientific item* recommendation systems

## exclude

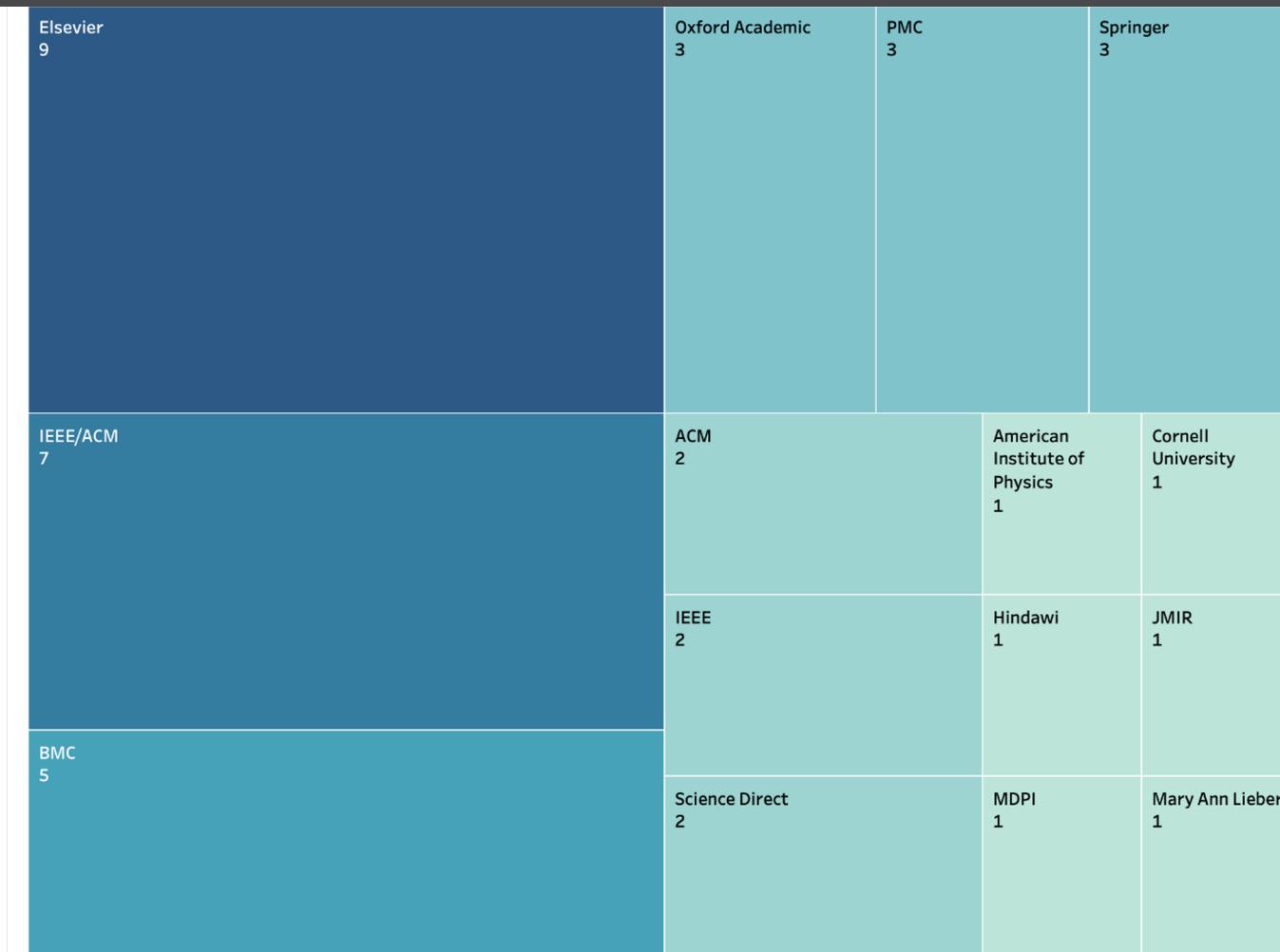
1. manuscripts written in other language than english
2. technical reports, master and PhD dissertation
3. surveys

## criteria of selection

1. clearly stated objectives, results and findings on the domain of knowledge
2. well-presented and justified arguments
3. well-referenced with a minimum of 10 sources

# Trends of a Glance: publisher

#articles

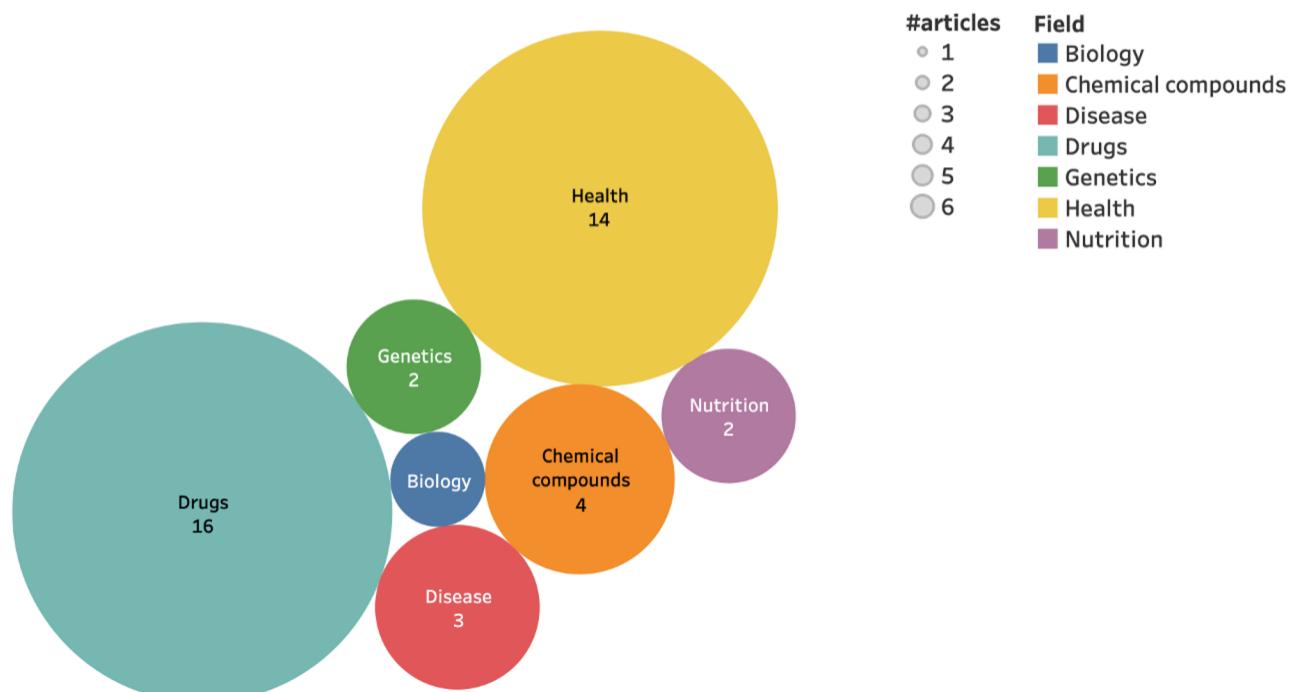
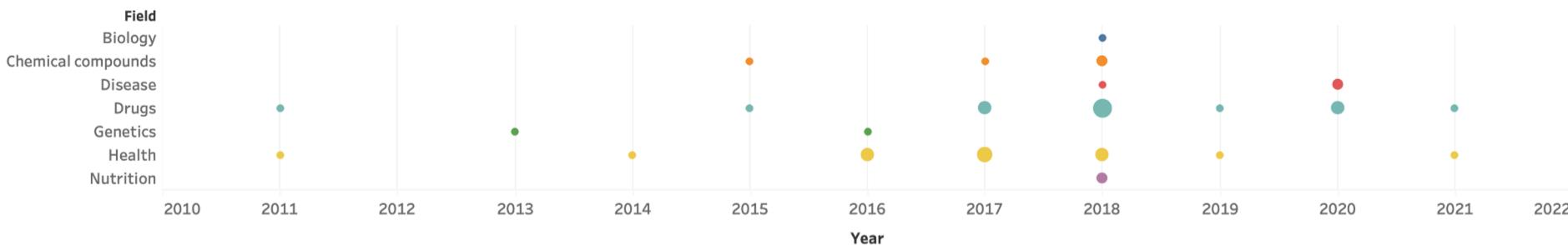


# Journal and conference

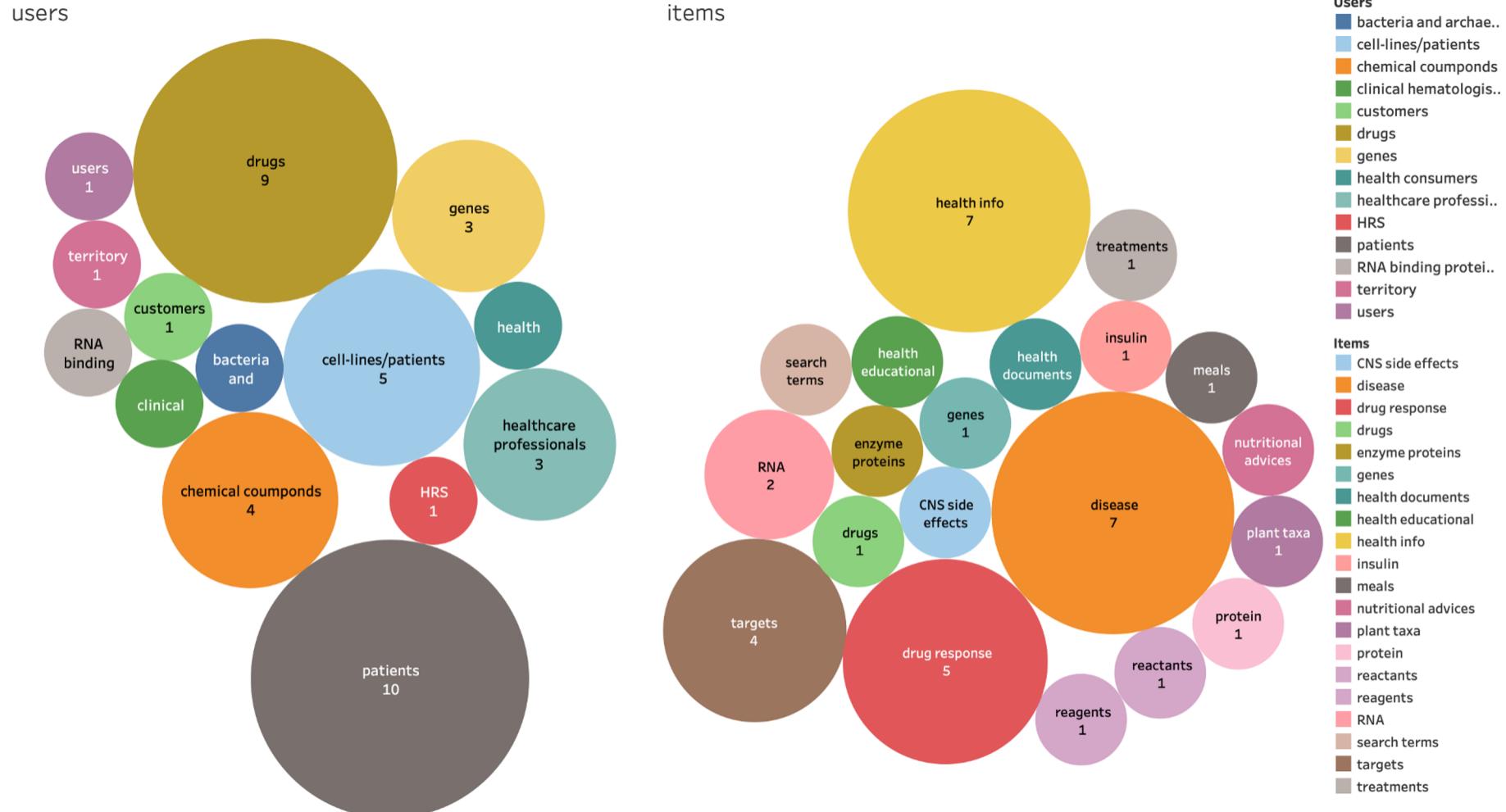


# Scientific fields

#articles



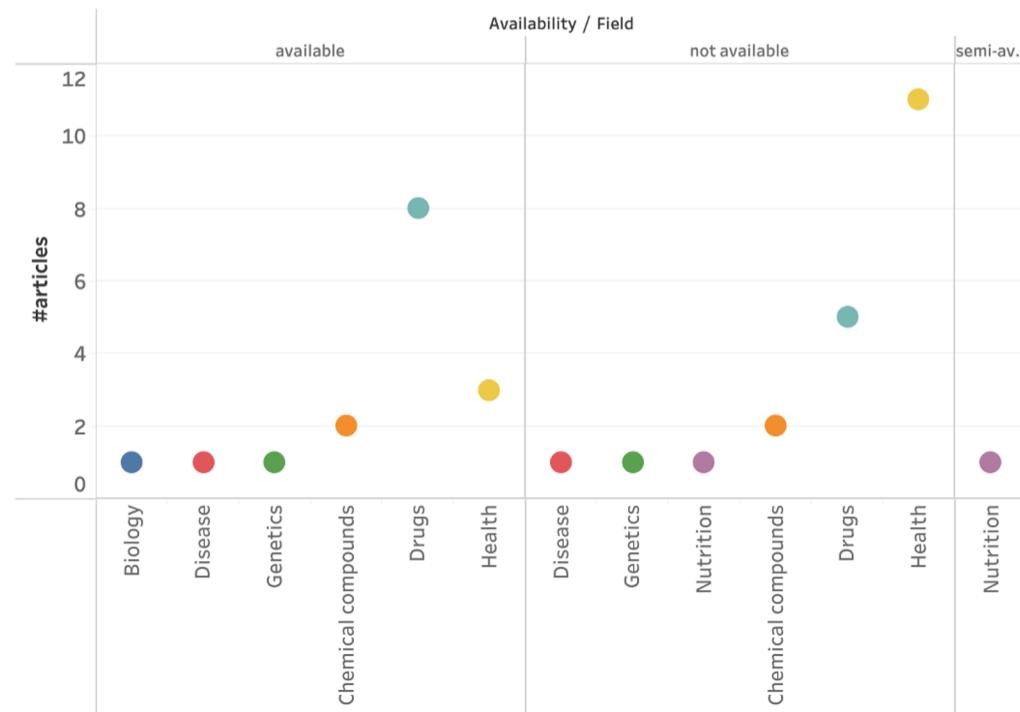
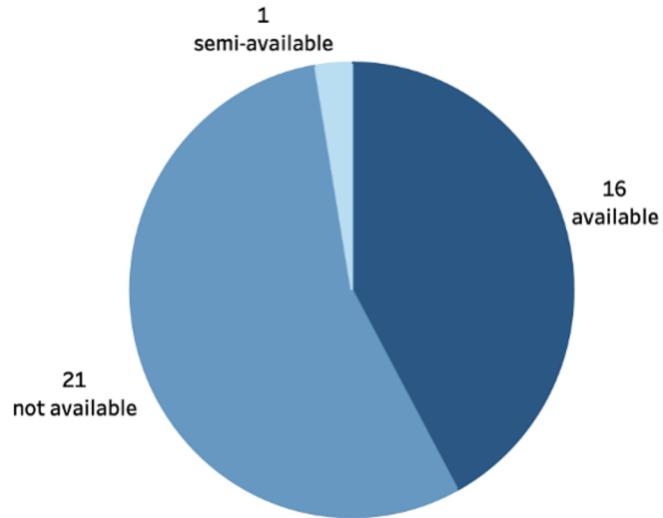
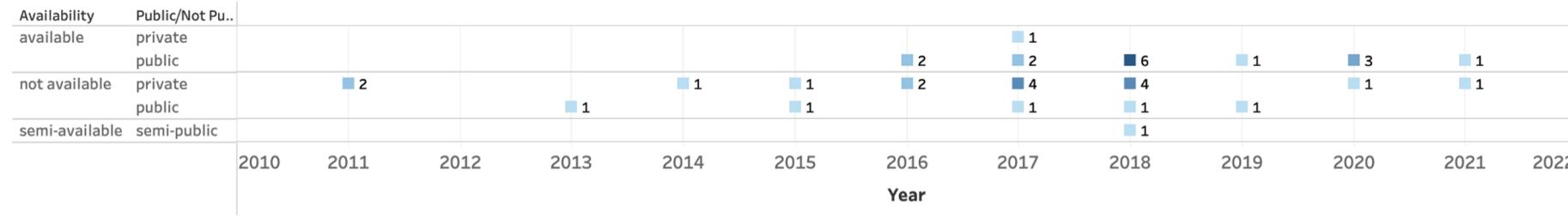
# Matrix Factorization



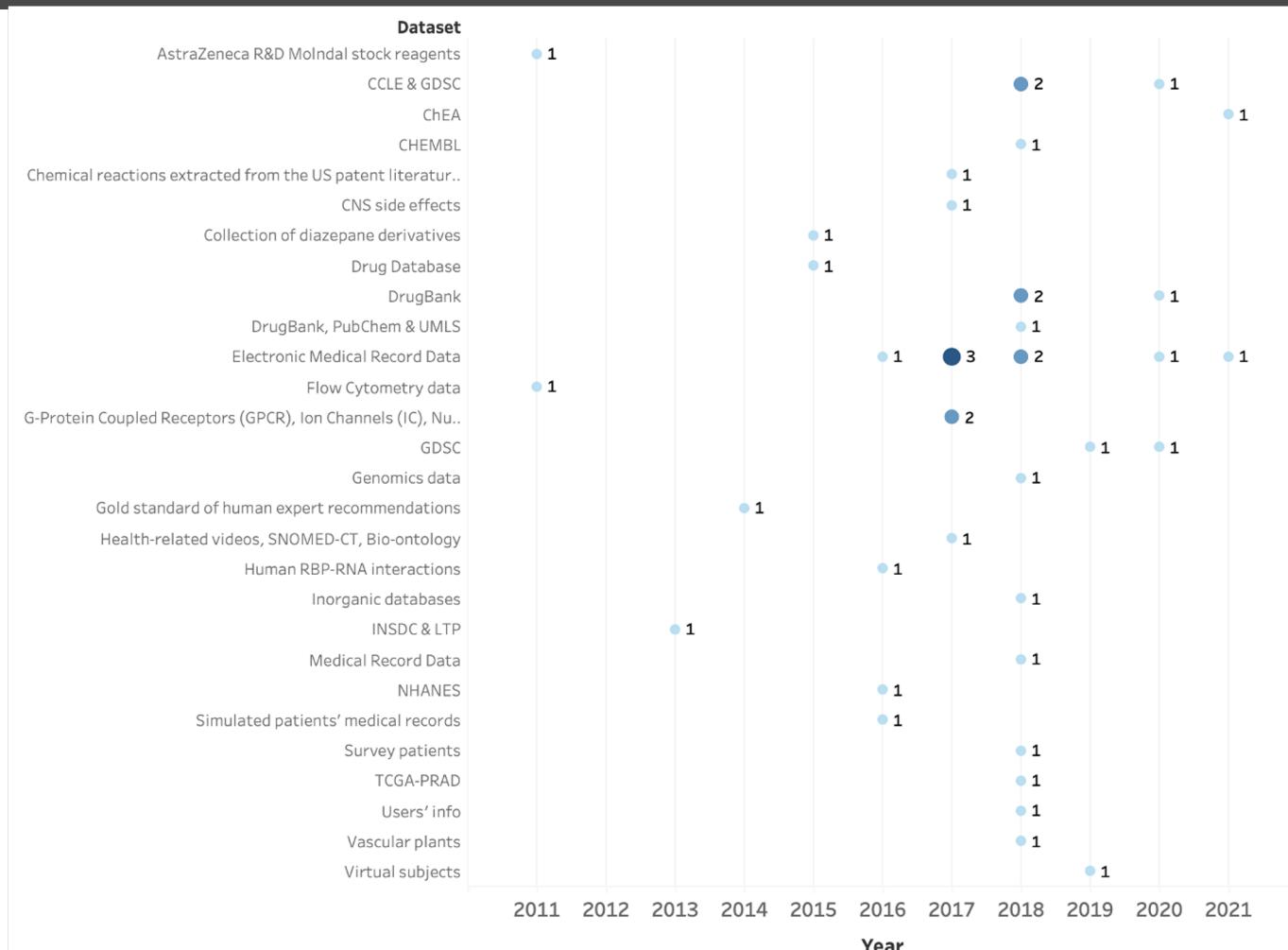
# tuple: < user, item >



# Availability of the dataset



# Source of the dataset



# Introduction to Named Entity Recognition (NER) and Named Entity Linking (NEL)

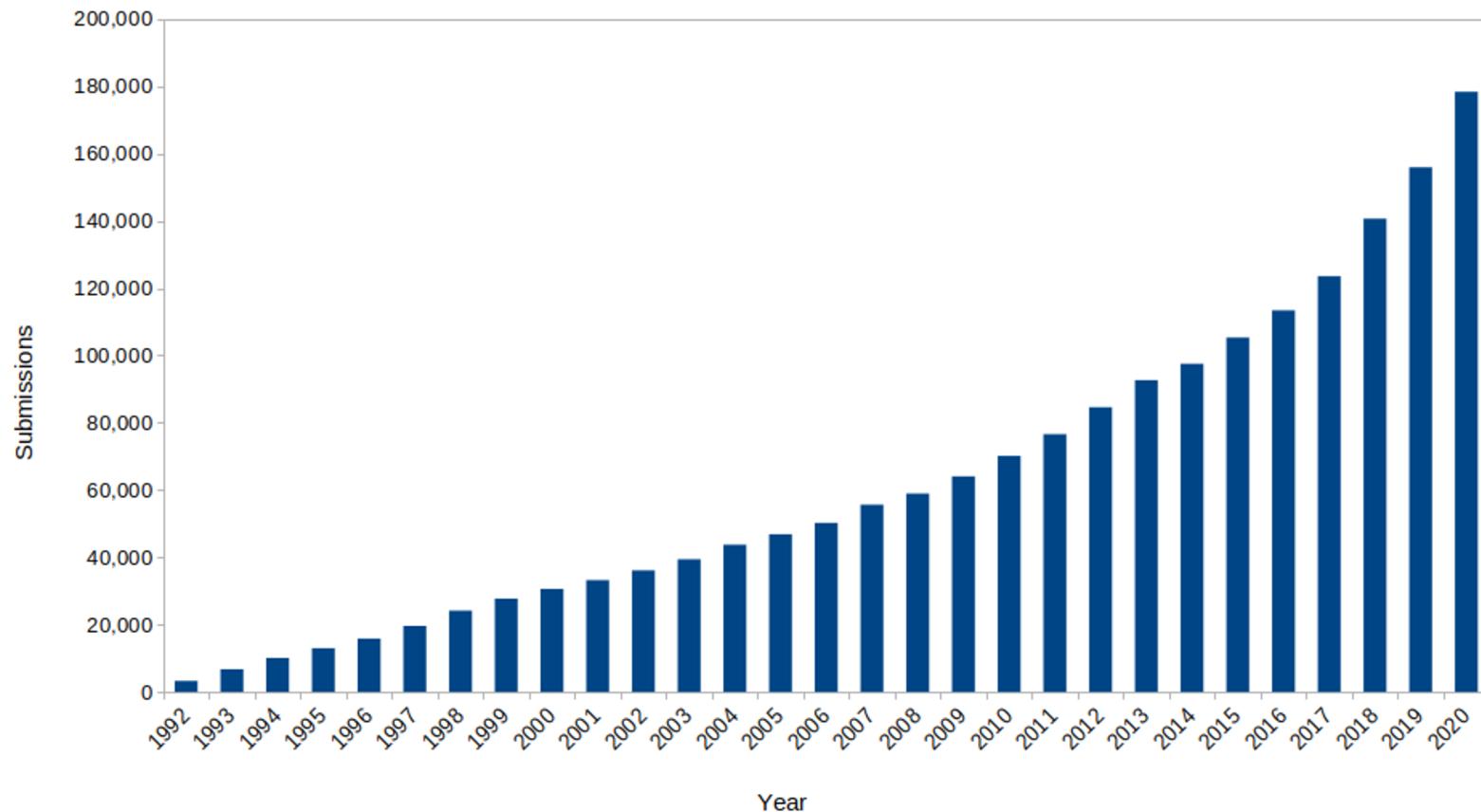
Pedro Ruas

Described in text in:

- published papers
- electronic health records
- clinical trials
- patents
- database entries
- ...

# Scientific/biomedical knowledge

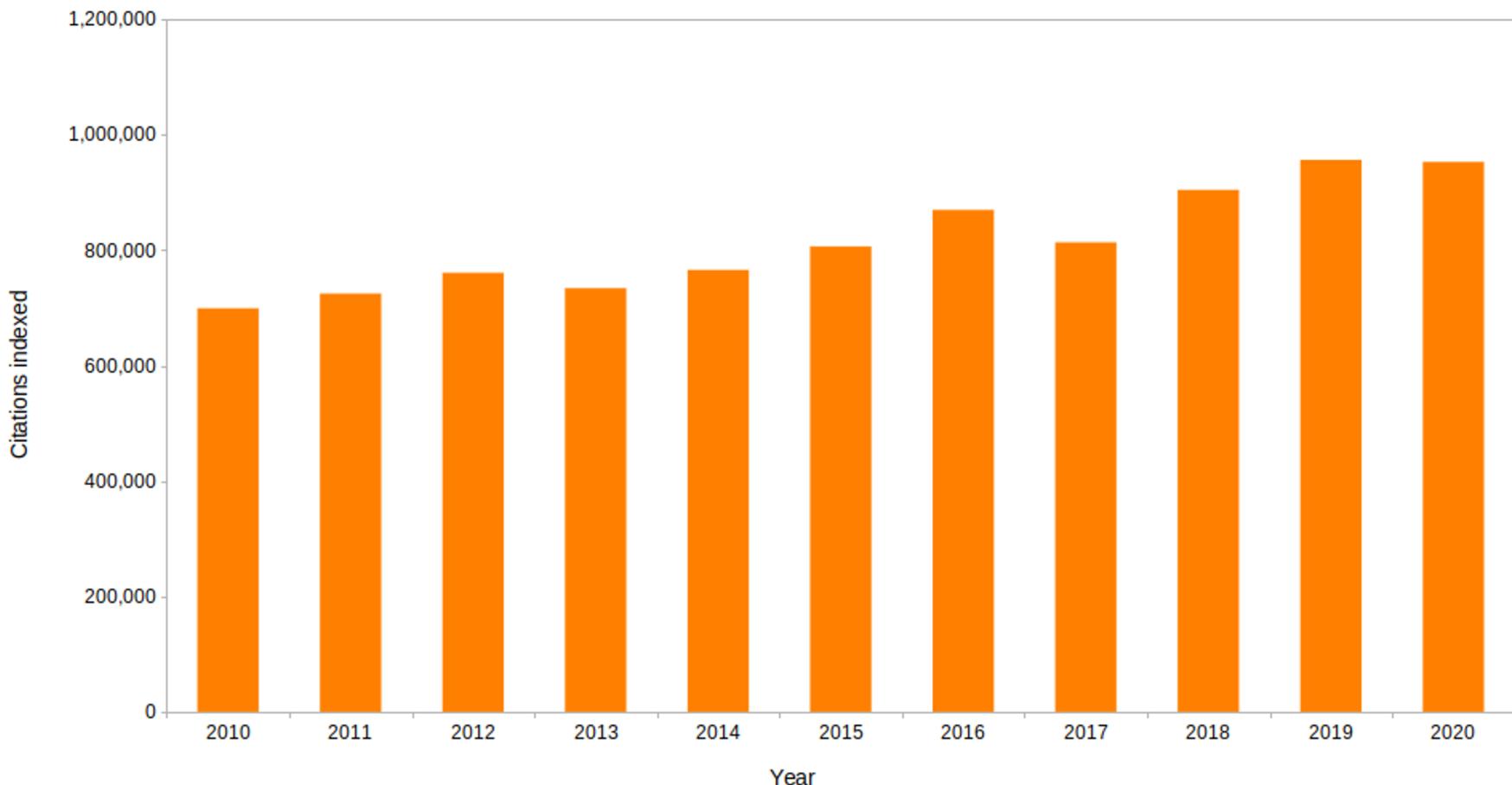
New submissions to arXiv by year<sup>1</sup>



<sup>1</sup>Based on: [https://arxiv.org/stats/monthly\\_submissions](https://arxiv.org/stats/monthly_submissions)

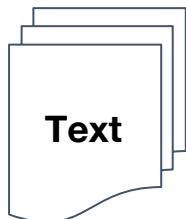
# Scientific/biomedical knowledge

Citations indexed to MEDILINE Pubmed by year<sup>1</sup>

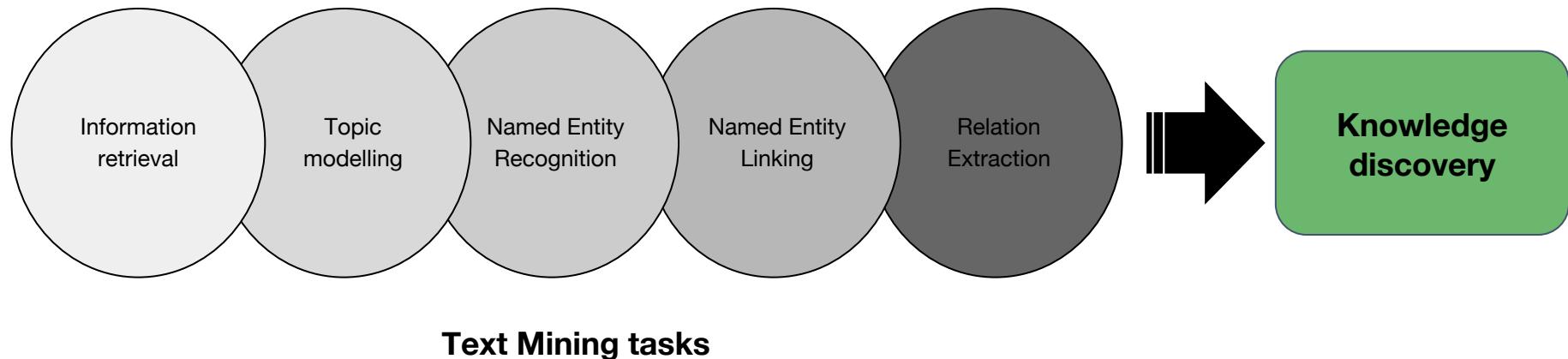
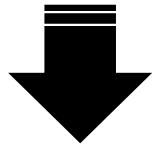


<sup>1</sup>Based on: [https://www.nlm.nih.gov/bsd/medline\\_pubmed\\_production\\_stats.html](https://www.nlm.nih.gov/bsd/medline_pubmed_production_stats.html)

# Text Mining



Text Mining bridges the gap between natural language (text) and knowledge



# Named Entity Recognition

## Definition

Task introduced in the MUC-6 evaluation (1995):

«*Named Entity (NE) -- Insert SGML tags into the text to mark each string that represents a person, organization, or location name, or a date or time stamp, or a currency or percentage figure.*»<sup>1</sup>

Another definition (2018):

«*Named Entity Recognition and Classification, an important sub-task of Information Extraction, points to **identify** and **classify** members of rigid designators from data suited to different types of named entities such as organizations, persons, locations, etc.*»<sup>2</sup>

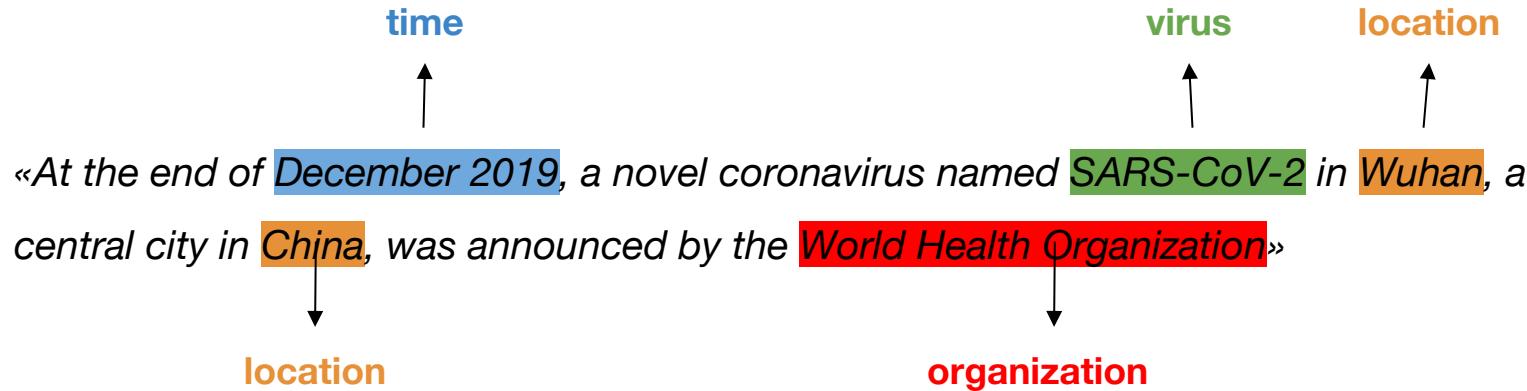
<sup>1</sup>B. M. Sundheim, "Overview of results of the MUC-6 evaluation," in *MUC6 '95: Proceedings of the 6th conference on Message understanding*, 1995, pp. 13–31, doi: <https://doi.org/10.3115/1072399.1072402>.

<sup>2</sup>A. Goyal, V. Gupta, and M. Kumar, "Recent Named Entity Recognition and Classification techniques: A systematic review," *Comput. Sci. Rev.*, vol. 29, pp. 21–43, 2018, doi: 10.1016/j.cosrev.2018.06.001.

# Named Entity Recognition

Definition

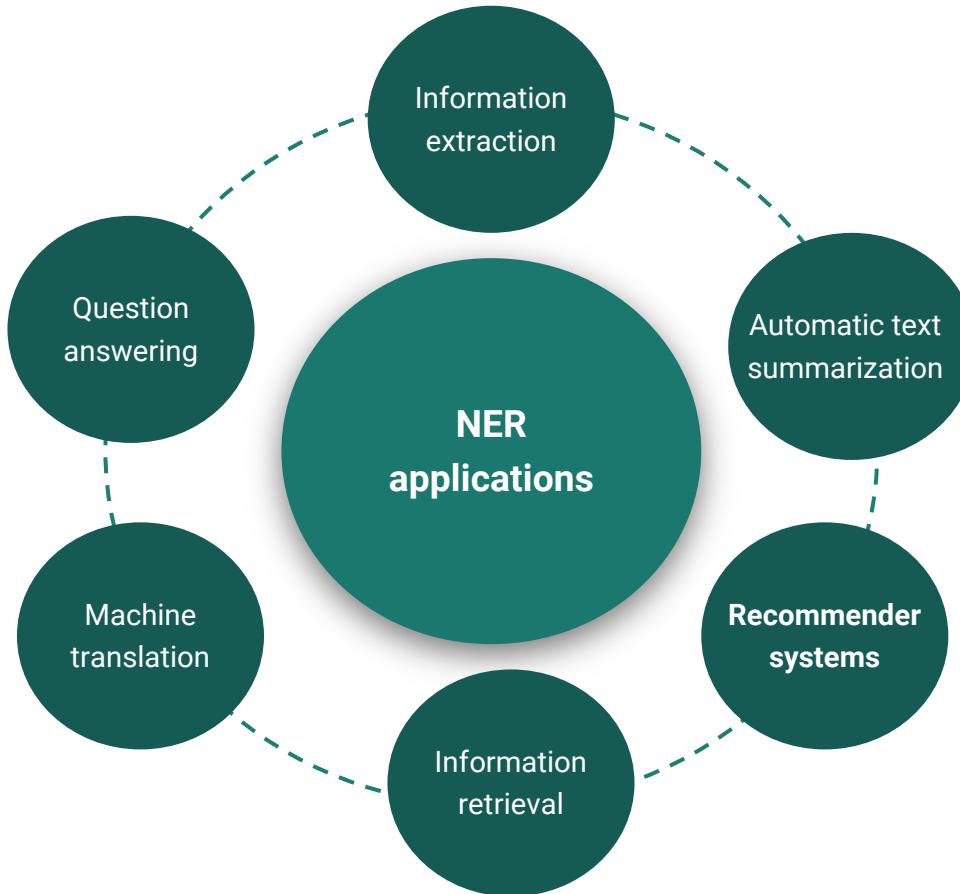
## Example



Entity	Begin	End	Category
"December 2019"	13	26	time
"SARS-CoV-2"	54	64	virus
"Wuhan"	68	73	location
"China"	93	98	location
"World Health Organization"	121	146	organization

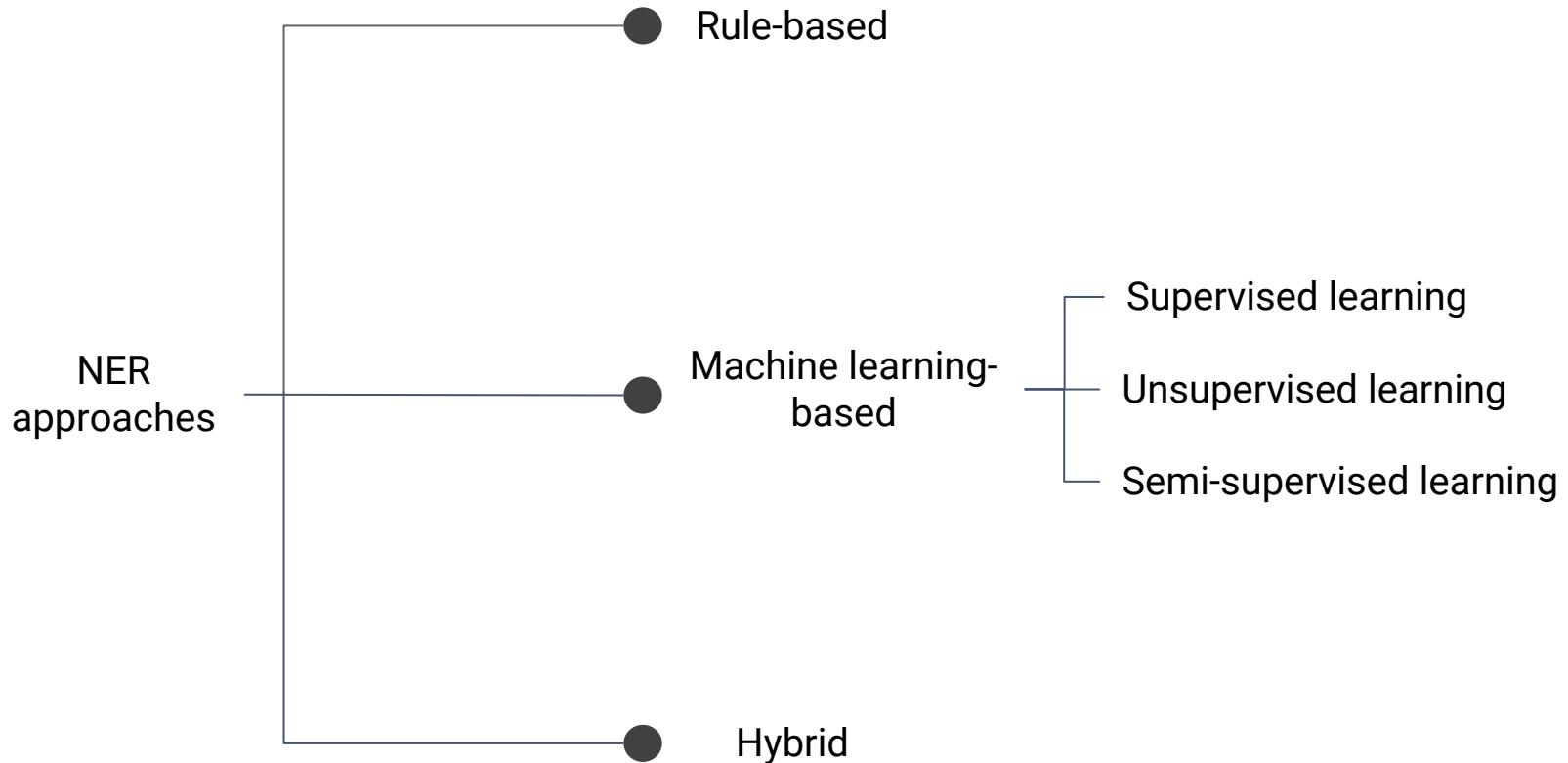
# Named Entity Recognition

## Applications



# Named Entity Recognition

## Types of systems

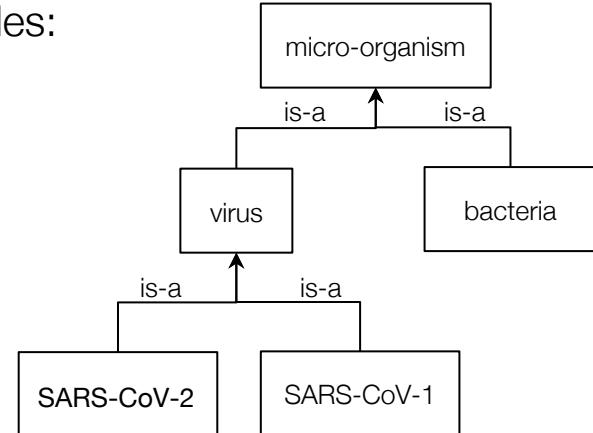


Based on A. Goyal, V. Gupta, and M. Kumar, "Recent Named Entity Recognition and Classification techniques: A systematic review," *Comput. Sci. Rev.*, vol. 29, pp. 21–43, 2018, doi: 10.1016/j.cosrev.2018.06.001.

# Knowledge Bases

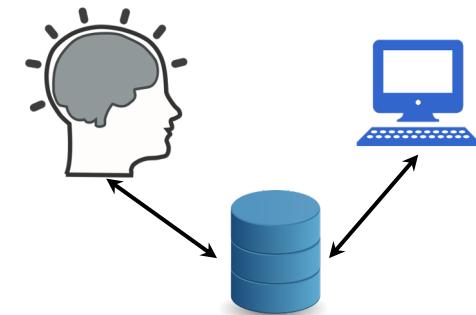
Formal representation of the reality or a part of it, which includes:

- concepts
- definitions
- attributes
- relations between concepts



## Advantages

- shared understanding of reality/knowledge
- integration of knowledge
- accessible by both computer reasoning and humans

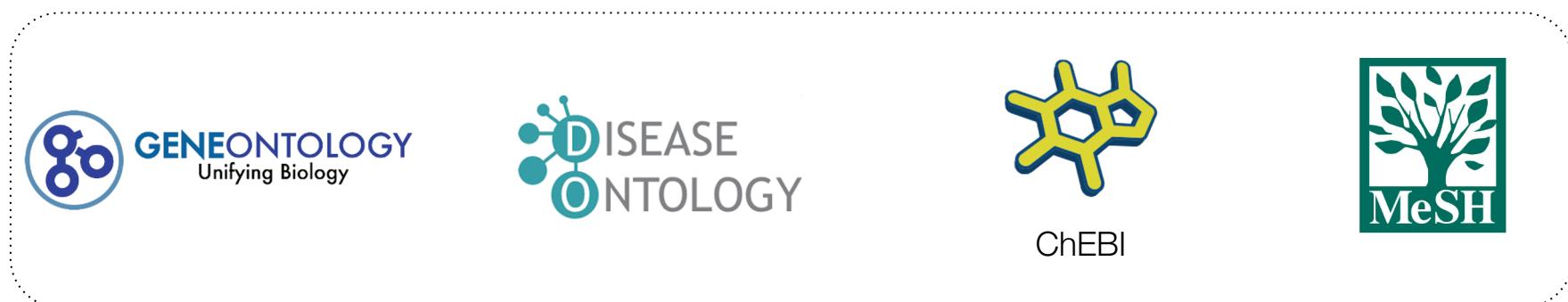


# Knowledge Bases

## General domain



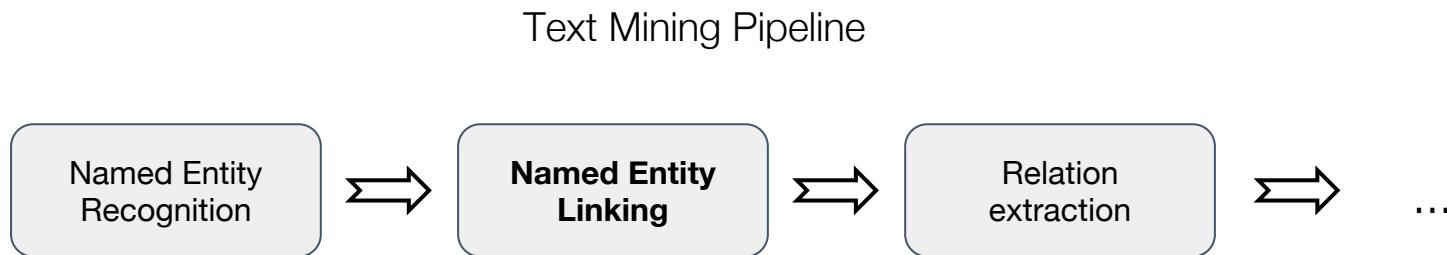
## In the biomedical domain



# Named Entity Linking (NEL)

## Definition

«**Entity Linking**, also referred to as *record linkage* or *entity resolution*, involves aligning a textual mention of a **named-entity** to an appropriate **entry in a knowledge base**, which may or may not contain the entity.»<sup>1</sup>

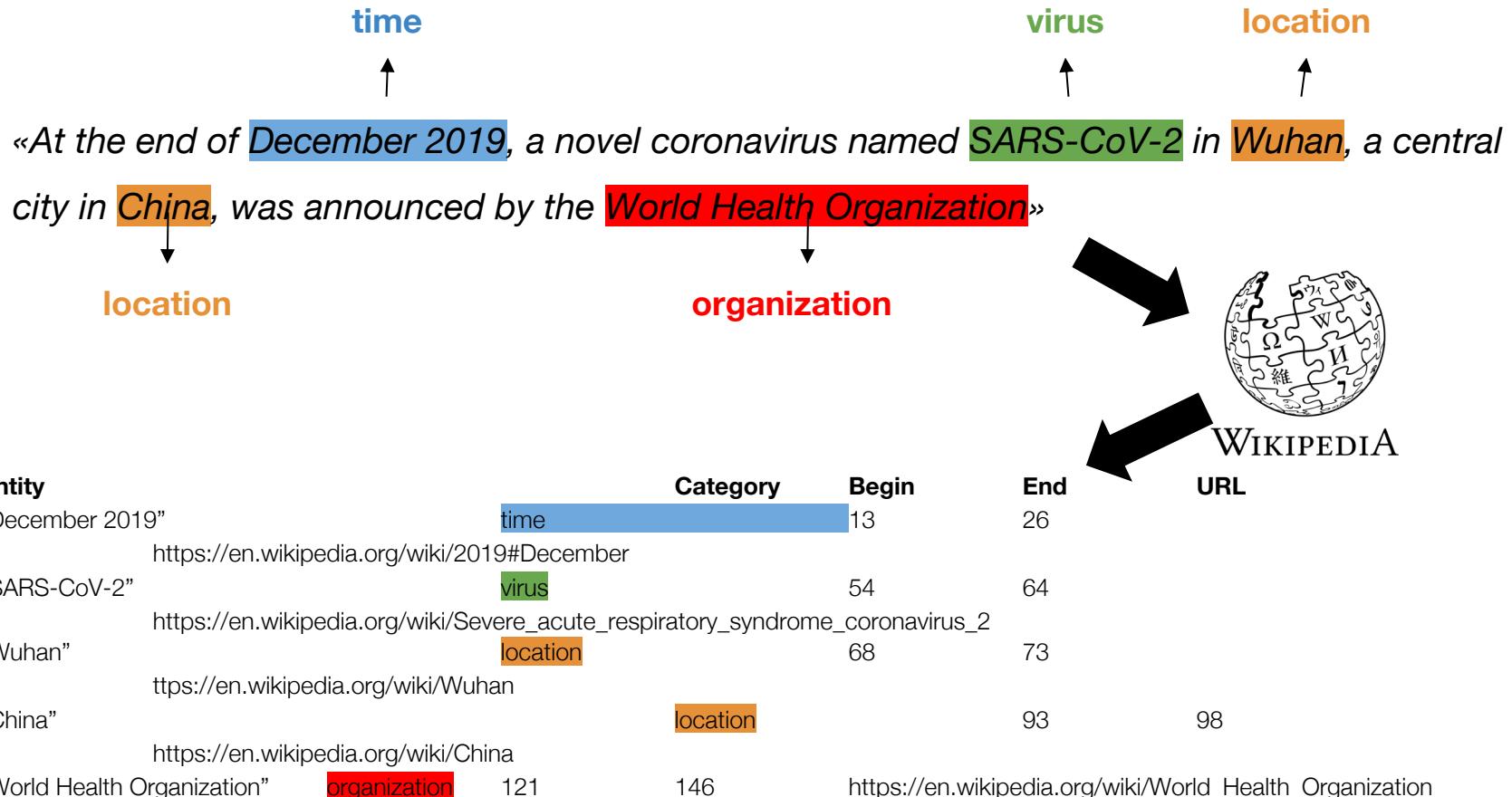


<sup>1</sup>D. Rao, P. McNamee, and M. Dredze, "Entity Linking: Finding Extracted Entities in a Knowledge Base," in *Multi-source, Multilingual Information Extraction and Summarization. Theory and Applications of Natural Language Processing.*, P. J. Poibeau T., Saggion H., Ed. Springer, Berlin, Heidelberg, 2013, pp. 93–115.

# Named Entity Linking (NEL)

## Definition

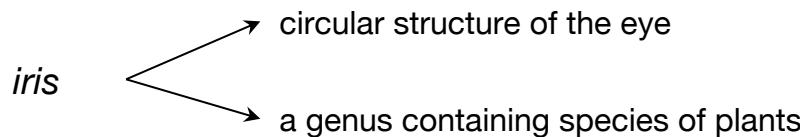
## Example



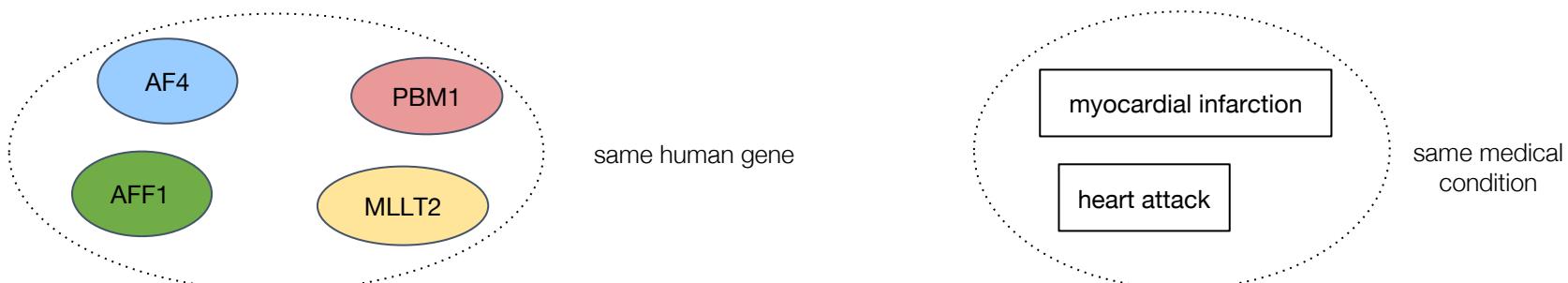
# Named Entity Linking (NEL)

## Challenges

- **Ambiguity**



- **Entity name variations** (abbreviations, synonyms, acronyms)

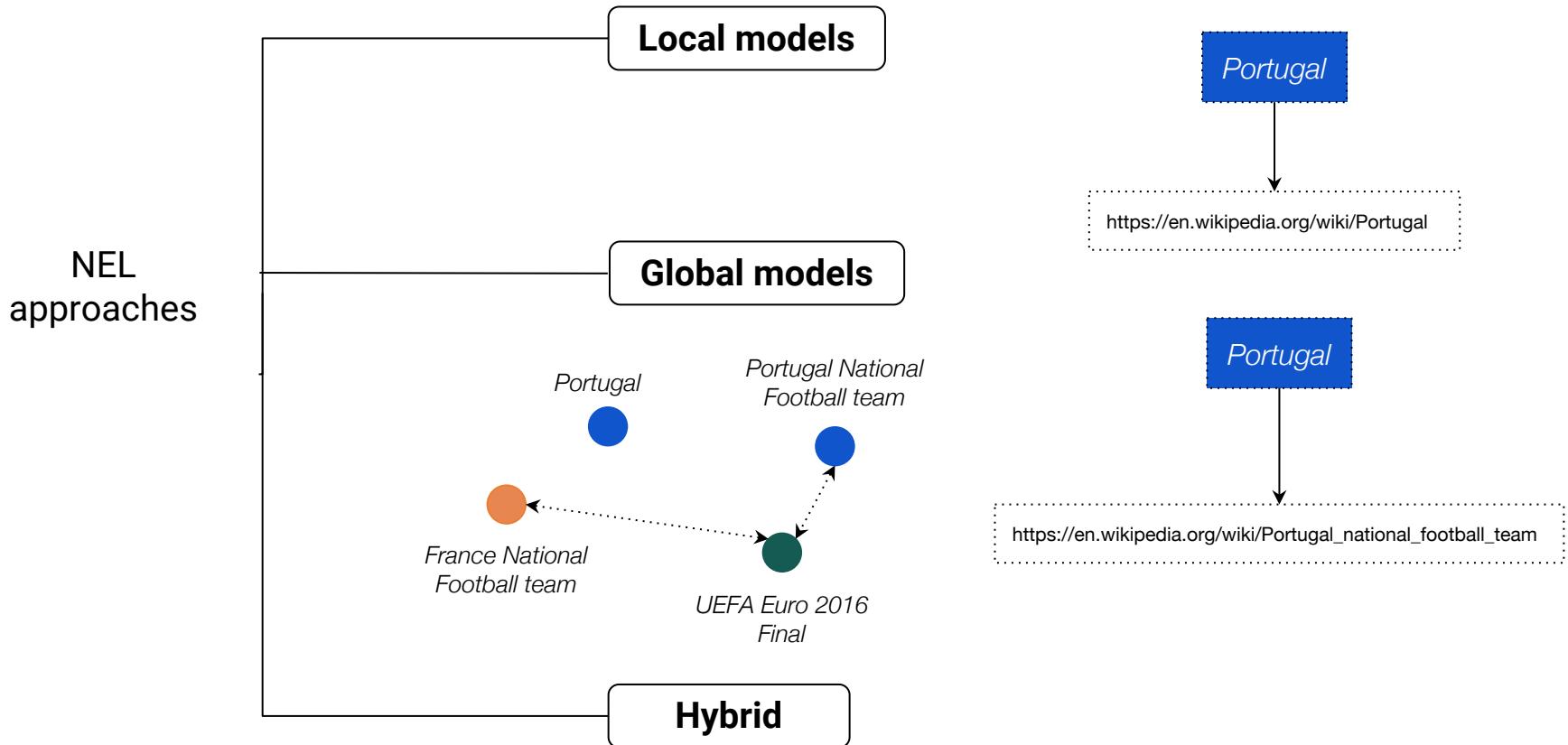


- **Incomplete ontologies/KBs**

# Named Entity Linking (NEL)

Types of systems

«Portugal defeated France 1–0 at UEFA Euro 2016 Final»



# NER + NEL + Recommender systems

## What is the role of Text Mining in Recommender systems?

«(...) text mining techniques can be exploited for the development of recommender systems (...) can be applied to detect user preferences (**user profiling**) and also to **extract context data.**»<sup>1</sup>

<sup>1</sup>Y. Betancourt and S. Ibarri, "Use of text mining techniques for recommender systems," in ICEIS 2020 - Proceedings of the 22nd International Conference on Enterprise Information Systems, 2020, vol. 1, no. Iceis, pp. 780-787, doi: 10.5220/0009576507800787.

# NER + NEL + Recommender systems

Ref	Field	RS type	Role of NER/NEL	NER/NEL Tool	Ontologies
1	Videos	-	To extract content information from videos	-	-
2	News	Content-based	NER is used in tweets and external sources of news articles for creating better users' profiles, improving the recommendations	-	-
3	Movies	Content-based	To identify most relevant context found in text related to the movies, to create users' and items' profiles	DBpedia Spotlight, Wikipedia Mine, TAGME	DBpedia, Wikipedia
4	Books	Content-based	To identify most relevant context found in text related to the books, to create users' and items' profiles	TAGME	DBpedia

1. Q. Qi and J. Dong, "Named entity recognition in titles of Chinese videos from the web," *Proc. - 2011 IEEE Int. Conf. Comput. Sci. Autom. Eng. CSAE 2011*, vol. 4, pp. 220–224, 2011, doi: 10.1109/CSAE.2011.5952838.
2. F. Abel, Q. Gao, G. J. Houben, and K. Tao, "Analyzing user modeling on Twitter for personalized news recommendations" *Lect. Notes Comput. Sci. (including Subser. Lect. Notes Artif. Intell. Lect. Notes Bioinformatics)*, vol. 6787 LNCS, pp. 1–12, 2011, doi: 10.1007/978-3-642-22362-4\_1.
3. C. Musto, G. Semeraro, P. Lops, and M. de Gemmis, "Combining distributional semantics and entity linking for context-aware content-based recommendation," *Lect. Notes Comput. Sci. (including Subser. Lect. Notes Artif. Intell. Lect. Notes Bioinformatics)*, vol. 8538, pp. 381–392, 2014, doi: 10.1007/978-3-319-08786-3\_34.
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# NER + NEL + Recommender systems

Ref	Field	RS type	Role of NER/NEL	NER/NEL Tool	Ontologies
5	Agro-business web pages	Collaborative-filtering	To extract entities from web pages to enrich the dataset	-	-
6	Agro-business web pages, movies	Collaborative-filtering	To extract entities from web pages to enrich the dataset	REMBRANDT, Stanford NER	Wikipedia
7	Dietary-related web pages, scientific text	-	To extract dietary concepts and recommendations from scientific sources	drNER	-
8	Teaching resources	-	To extract and link entities in the transcript of educational resources	Dandelion NER	DBpedia
9	Movies	Content-based	To find relevant entities mentioned in the user sentence in order to improve a dialog manager	-	Wikidata

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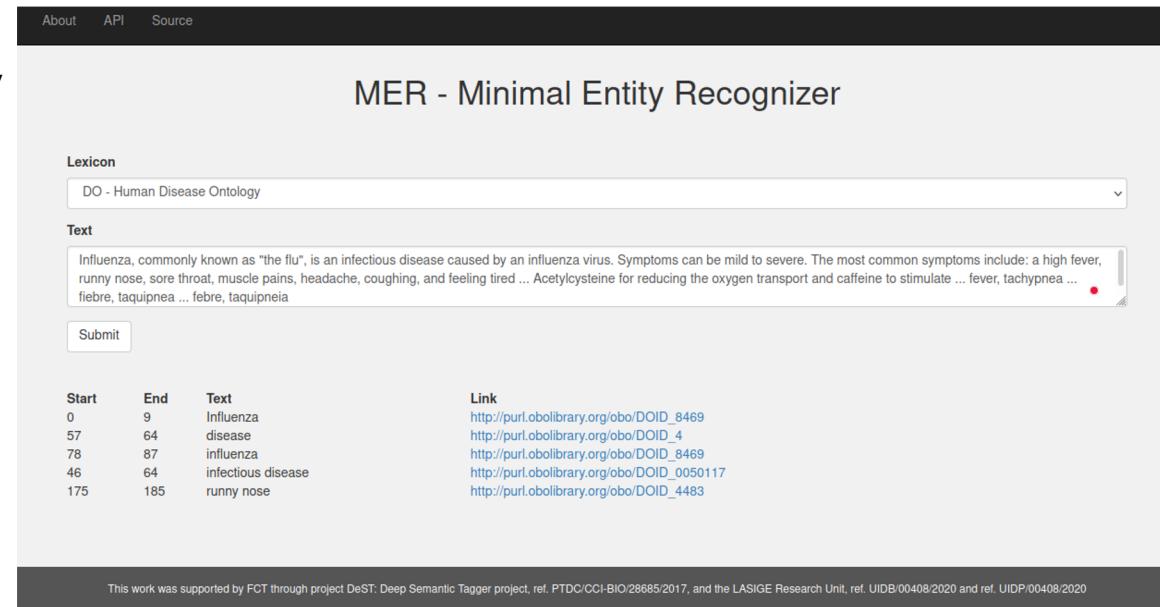
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Minimal Named Entity Recognizer<sup>1</sup>

- NER + NEL step
- text processing command-line tools *grep* and *awk*
- inverted recognition technique
- Python implementation: *merpy*



MER - Minimal Entity Recognizer

Lexicon

DO - Human Disease Ontology

Text

Influenza, commonly known as "the flu", is an infectious disease caused by an influenza virus. Symptoms can be mild to severe. The most common symptoms include: a high fever, runny nose, sore throat, muscle pains, headache, coughing, and feeling tired ... Acetylcysteine for reducing the oxygen transport and caffeine to stimulate ... fever, tachypnea ... fiebre, taquipnea ... febre, taquipnea

Submit

Start	End	Text	Link
0	9	Influenza	<a href="http://purl.obolibrary.org/obo/DOID_8469">http://purl.obolibrary.org/obo/DOID_8469</a>
57	64	disease	<a href="http://purl.obolibrary.org/obo/DOID_4">http://purl.obolibrary.org/obo/DOID_4</a>
78	87	influenza	<a href="http://purl.obolibrary.org/obo/DOID_8469">http://purl.obolibrary.org/obo/DOID_8469</a>
46	64	infectious disease	<a href="http://purl.obolibrary.org/obo/DOID_0050117">http://purl.obolibrary.org/obo/DOID_0050117</a>
175	185	runny nose	<a href="http://purl.obolibrary.org/obo/DOID_4483">http://purl.obolibrary.org/obo/DOID_4483</a>

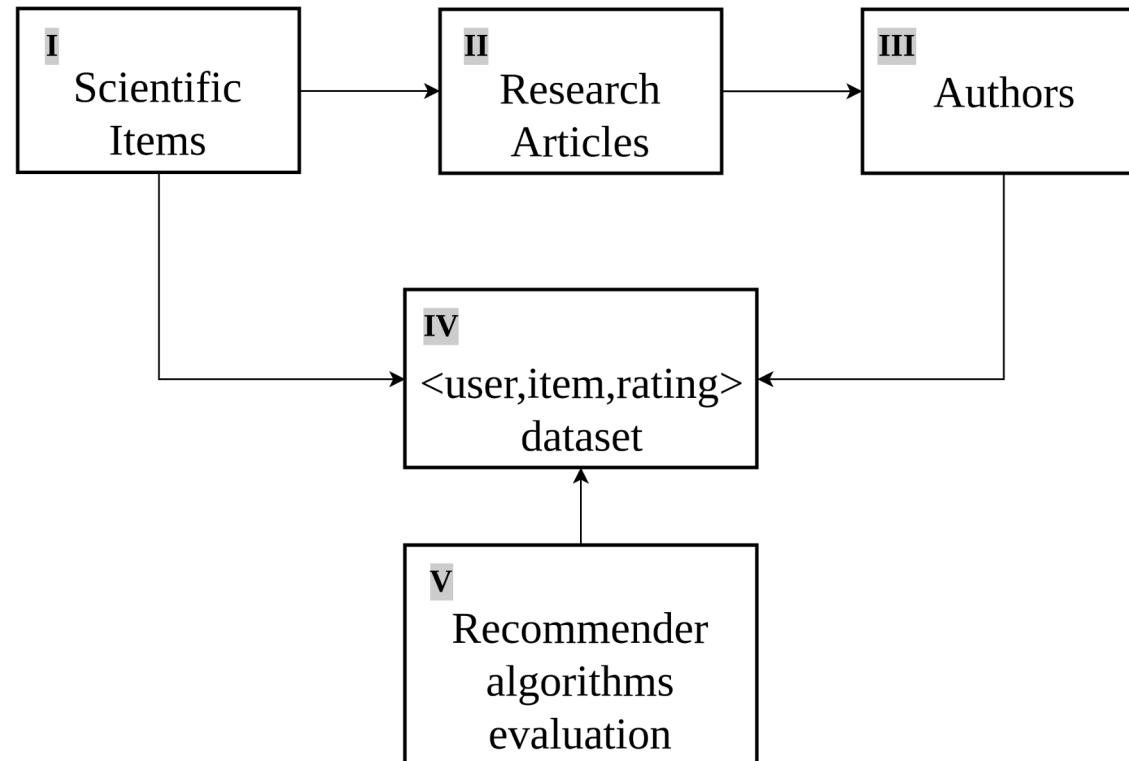
This work was supported by FCT through project DeST: Deep Semantic Tagger project, ref. PTDC/CCI-BIO/28685/2017, and the LASIGE Research Unit, ref. UIDB/00408/2020 and ref. UIDP/00408/2020

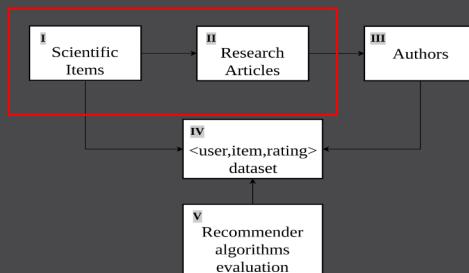
<sup>1</sup>F. M. Couto and A. Lamurias, "MER: a shell script and annotation server for minimal named entity recognition and linking," *J. Cheminform.*, vol. 10, no. 1, p. 58, Dec. 2018, doi: 10.1186/s13321-018-0312-9.

# LIterature Based RecommEndaTion of scienTific Items (LIBRETTI)

**Márcia Barros**

**Goal:** Create a **standard dataset** (user, item, rating) for recommender algorithms by extracting **implicit** information from the **scientific literature**





knowledge base with information about research articles mentioning the entities

EMBL-EBI Services Research Training About us

ChEBI Search Examples: iron\*, InChI1S/C14O/c1-3h2h14/h... ★★★ Advanced

Home Advanced Search Browse Documentation Download Tools About ChEBI Contact us Submit

ChEBI > Main

CHEBI:46195 - paracetamol

Main ChEBI Ontology Automatic Xrefs Reactions Pathways Models

paracetamol

ChEBI Name paracetamol

ChEBI ID CHEBI:46195

Definition A member of the class of phenols that is 4-aminophenol in which one of the hydrogens attached to the amino group has been replaced by an acetyl group.

Stars ★★★ This entity has been manually annotated by the ChEBI Team.

Secondary ChEBI IDs CHEBI:46191, CHEBI:2386

Supplier Information ChemicalBook:CB1413658, ChemicalBook:CB61261439, ChemicalBook:CB24796965, eMolecules:474380, eMolecules:27677450, MolPort:000-150-777, ZINC000013550868

Download Molfile XML SDF

- Find compounds which contain this structure
- Find compounds which resemble this structure
- Take structure to the Advanced Search

more structures >>

**Citations**

Cohen IV, Cirulli ET, Mitchell MW, Jonsson TJ, Yu J, Shah N, Spector TD, Guo L, Venter JC, Telenti A (2018) Acetaminophen (Paracetamol) Use Modifies the Sulfation of Sex Hormones. *EBioMedicine* 28, 316-323 [PubMed:29398597]

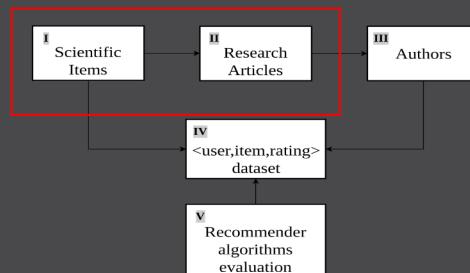
[show Abstract]

Lee WM (2017) Acetaminophen (APAP) hepatotoxicity-Isn't it time for APAP to go away? *Journal of hepatology* 67, 1324-1331 [PubMed:28734939]

[show Abstract]

Sawaguchi A, Sasaki K, Miyanaga K, Nakayama M, Nagasue M, Shimoda M (2016) Rapid absorption of diclofenac and acetaminophen after their oral administration to cattle. *The Journal of veterinary medical science* 78, 1481-1485 [PubMed:27320817]

[show Abstract]



## NER + NEL



## Research Paper

**Acetaminophen (Paracetamol) Use Modifies the Sulfation of Sex Hormones**

Isaac V. Cohen <sup>a,b</sup>, Elizabeth T. Cirulli <sup>a</sup>, Matthew W. Mitchell <sup>c</sup>, Thomas J. Jonsson <sup>c</sup>, James Yu <sup>a</sup>, Naisha Shah <sup>a</sup>, Tim D. Spector <sup>d</sup>, Lining Guo <sup>c</sup>, J. Craig Venter <sup>a,e</sup>, Amalio Telenti <sup>b,e,\*</sup>

<sup>a</sup> Human Longevity, Inc., San Diego, CA, USA

<sup>b</sup> Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, San Diego, CA, USA

<sup>c</sup> Metabolon, Inc., Durham, NC, USA

<sup>d</sup> Department of Twin Research and Genetic Epidemiology, King's College London, London, UK

<sup>e</sup> J. Craig Venter Institute, La Jolla, CA, USA

**ARTICLE INFO****Article history:**

Received 30 November 2017

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**Keywords:**  
Metabolome  
Mendelian randomization  
Sulfotransferases  
sult2a1

**ABSTRACT**

**Background:** Acetaminophen [paracetamol] is one of the most common medications used for management of pain in the world. There is lack of consensus about the mechanism of action, and concern about the possibility of adverse effects on reproductive health.

**Methods:** We first established the metabolome profile that characterizes use of acetaminophen, and we subsequently trained and tested a model that identified metabolomic differences across samples from 455 individuals with and without acetaminophen use. We validated the findings in a European ancestry adult twin cohort of 1880 individuals (TwinsUK), and in a study of 1235 individuals of African American and Hispanic ancestry. We used genomics to elucidate the mechanisms targeted by acetaminophen.

**Findings:** We identified a distinctive pattern of depletion of sulfated sex hormones with use of acetaminophen across all populations. We used a Mendelian randomization approach to characterize the role of Sulfotransferase Family 2A Member 1 (SULT2A1) as the site of the interaction. Although CYP3A7-CYP3A51P variants also modified levels of some sulfated sex hormones, only acetaminophen use phenocopied the effect of genetic variants of SULT2A1. Overall, acetaminophen use, age, gender and SULT2A1 and CYP3A7-CYP3A51P genetic variants are key determinants of variation in levels of sulfated sex hormones in blood. The effect of taking acetaminophen on sulfated sex hormones was roughly equivalent to the effect of 35 years of aging.

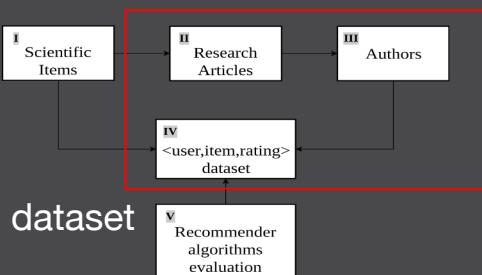
**Interpretation:** These findings raise concerns of the impact of acetaminophen use on hormonal homeostasis. In addition, it modifies views on the mechanism of action of acetaminophen in pain management as sulfated sex hormones can function as neurosteroids and modify nociceptive thresholds.

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Chemical compounds  
chEBI ID: **CHEBI:46195**

# LIBRETTI

From the articles to the recommendation dataset



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Research Paper

Acetaminophen (Paracetamol) Use Modifies the Sulfation of Sex Hormones

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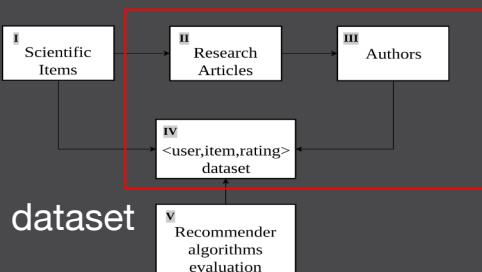
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User	Item	Rating
Isaac Cohen	Paracetamol	1
Elizabeth Cirulli	Paracetamol	1
Matthew Mitchell	Paracetamol	1
Thomas Jonsson	Paracetamol	1
James Yu	Paracetamol	1
Naisha Shah	Paracetamol	1
Tim Spector	Paracetamol	1
Lining Guo	Paracetamol	1
Craig Venter	Paracetamol	1
Amilio Telenti	Paracetamol	1

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**ELSEVIER**

Research Paper

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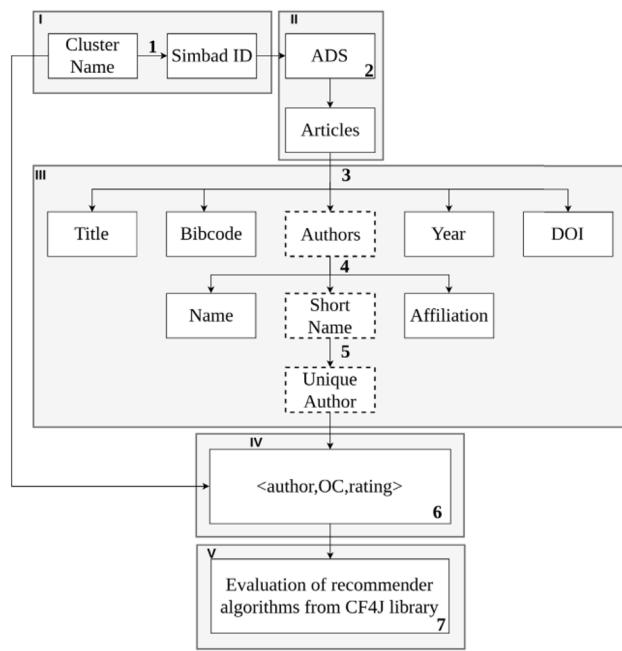
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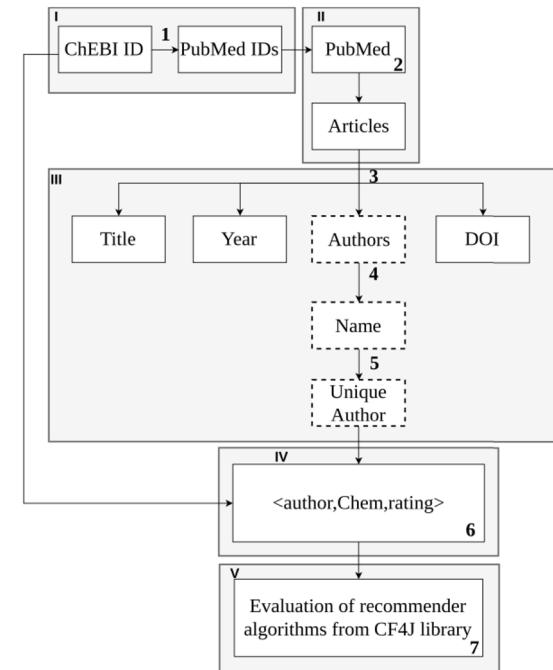
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User	Item	Rating	year
Isaac Cohen	Paracetamol	1	2018
Elizabeth Cirulli	Paracetamol	1	2018
Matthew Mitchell	Paracetamol	1	2018
Thomas Jonsson	Paracetamol	1	2018
James Yu	Paracetamol	1	2018
Naisha Shah	Paracetamol	1	2018
Tim Spector	Paracetamol	1	2018
Lining Guo	Paracetamol	1	2018
Craig Venter	Paracetamol	1	2018
Amalio Telenti	Paracetamol	1	2018

### Astronomy



### Chemistry



## COVID-19

---



NER+NEL

---

CHEBI

---

Gene Ontology

---

Disease Ontology

---

Human Phenotype Ontology

---

<User, Item,  
Rating>

CORD-19 dataset

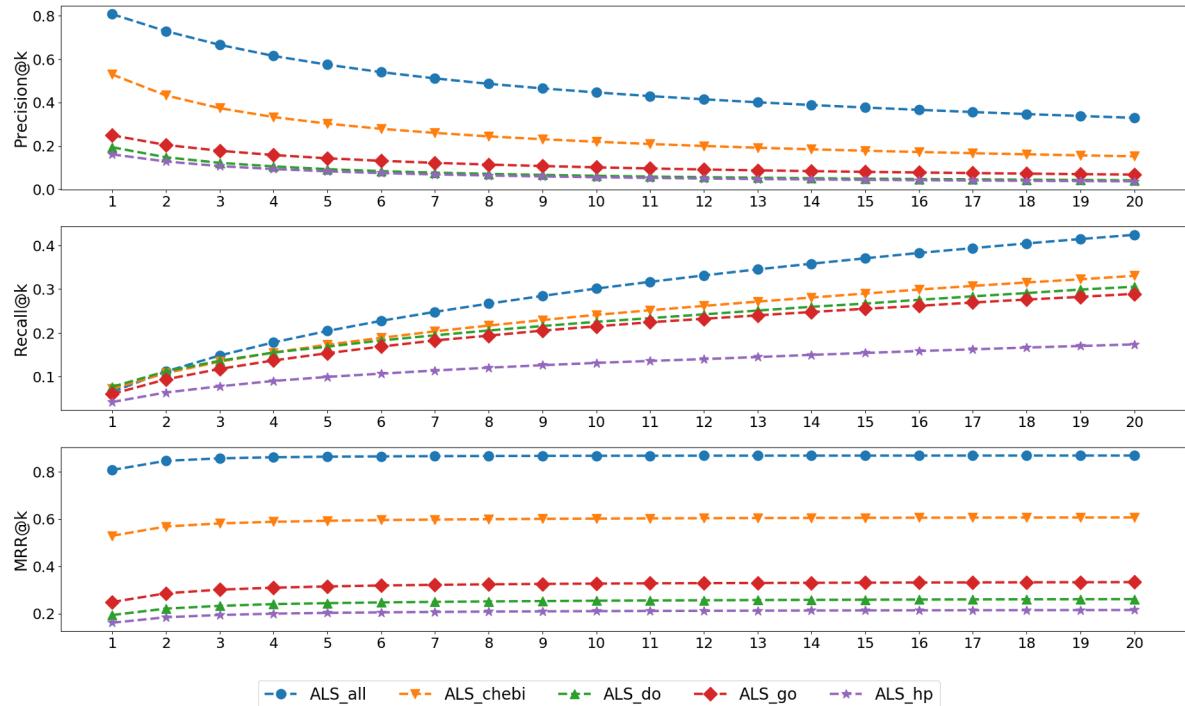
Items from multi scientific fields

Recommendation dataset

Barros, M. A., Lamurias, A., Sousa, D. F., Ruas, P., & Couto, F. M. (2020). COVID-19: A Semantic-Based Pipeline for Recommending Biomedical Entities. Proceedings of the 1st Workshop on NLP for COVID-19 (Part 2) at EMNLP 2020

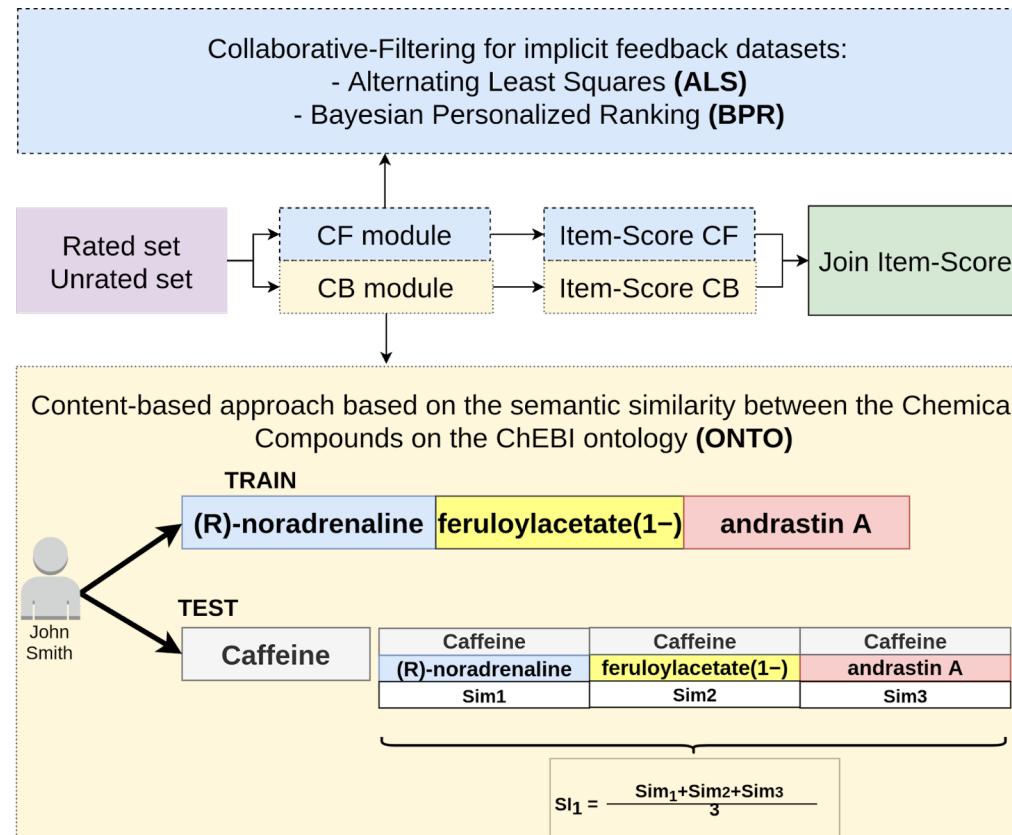
## Application fields

Using ontologies from different fields in the NER phase, we improve the results for state-of-the-art collaborative-filtering recommender systems applied to the dataset created.

**COVID-19**

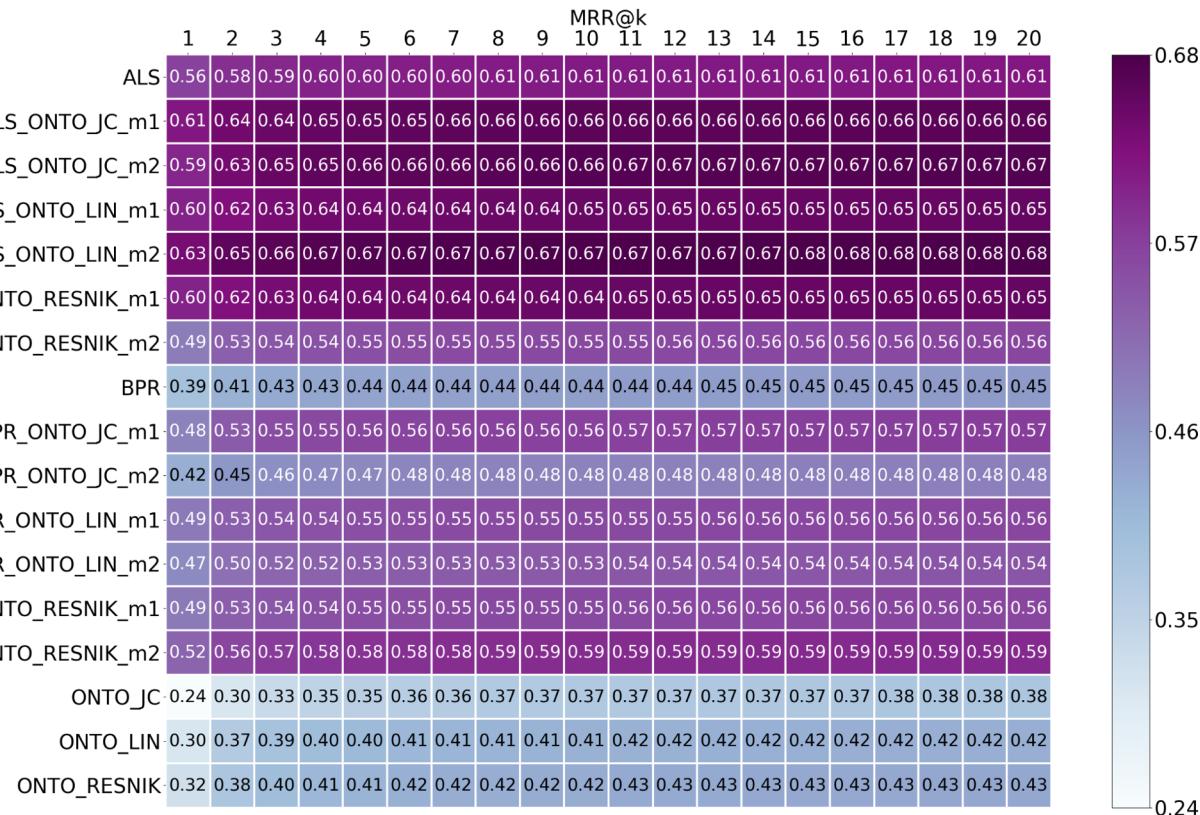
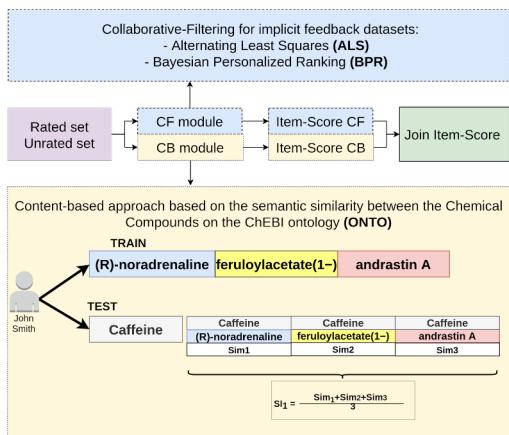
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# ONTO



Barros, Marcia, Andre Moitinho, and Francisco M. Couto. "Hybrid semantic recommender system for chemical compounds in large-scale datasets." *Journal of cheminformatics*. 13.1 (2021): 1-18.

# ONTO

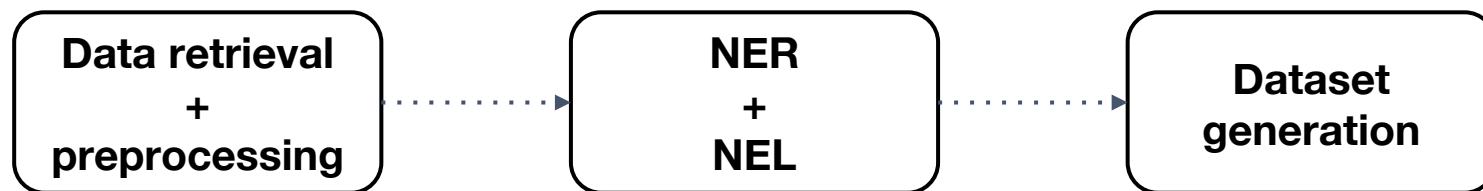


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# PART 2

# How to build a scientific recommendation dataset?

Tutorial sections



Source: >> **git clone git@github.com:lasigeBioTM/RecSys.Scifi.tutorial.git**

# THANK YOU!!!