# RecSys.Scifi: RECOMMENDER SYSTEMS DATASETS IN SCIENTIFIC FIELDS

KDD2021 Lecture-style Tutorial

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# Team

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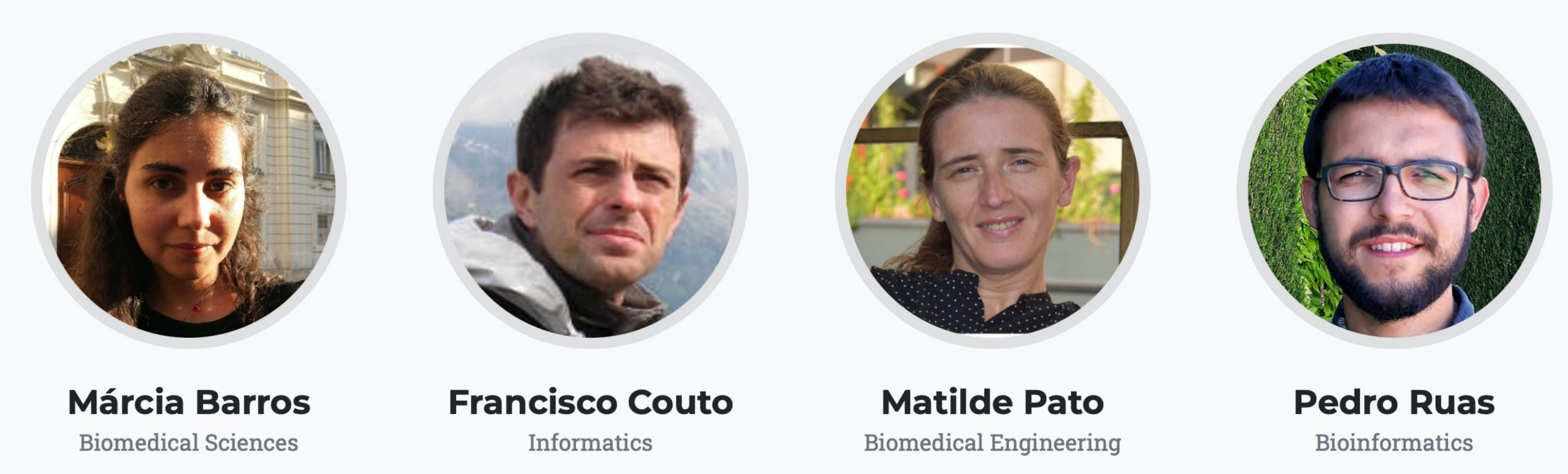

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https://lasigebiotm.github.io/RecSys.Scifi/

# Outline

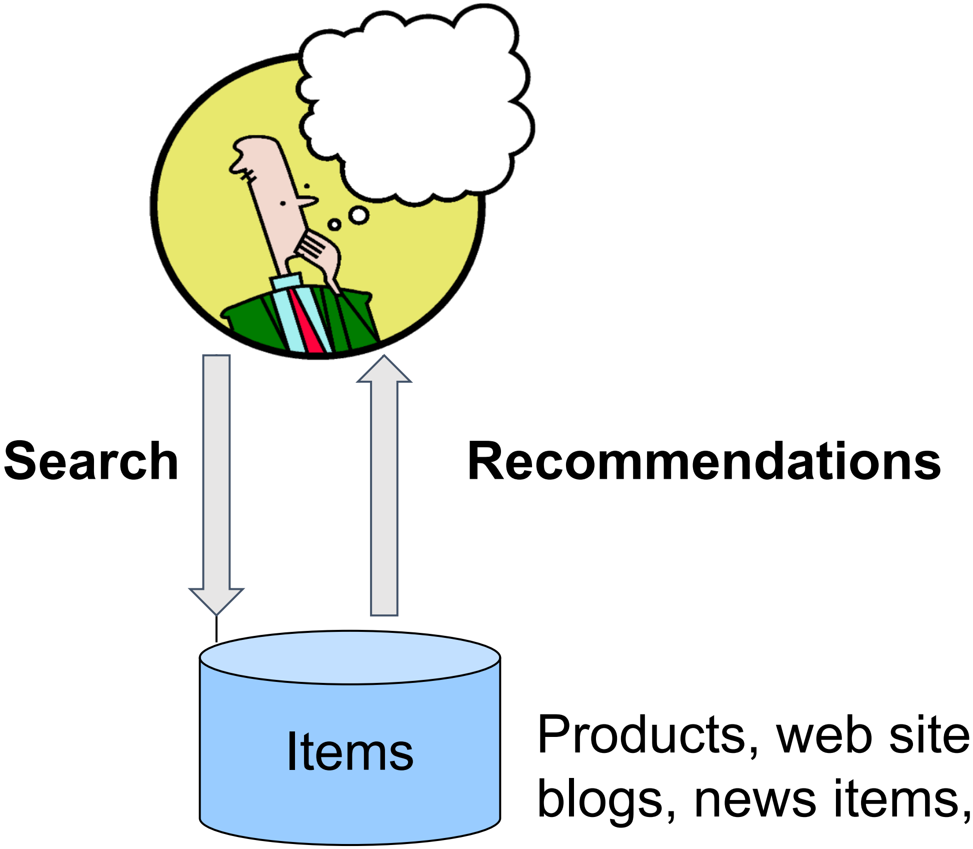
- PART 1
  - Introduction to Recommender Systems
  - Scientific recommender systems (state-of-the-art)
  - Introduction to Named Entity Recognition (NER) and Named Entity Linking (NEL)
  - LIterature Based RecommEndaTion of ScienTific Items LIBRETTI
- PART 2
  - Hands-on Labs – *How to build a scientific recommendation dataset?*
- PART 3
  - Open discussion

# PART 1

# Introduction to Recommender Systems

Francisco M. Couto

# Recommendations

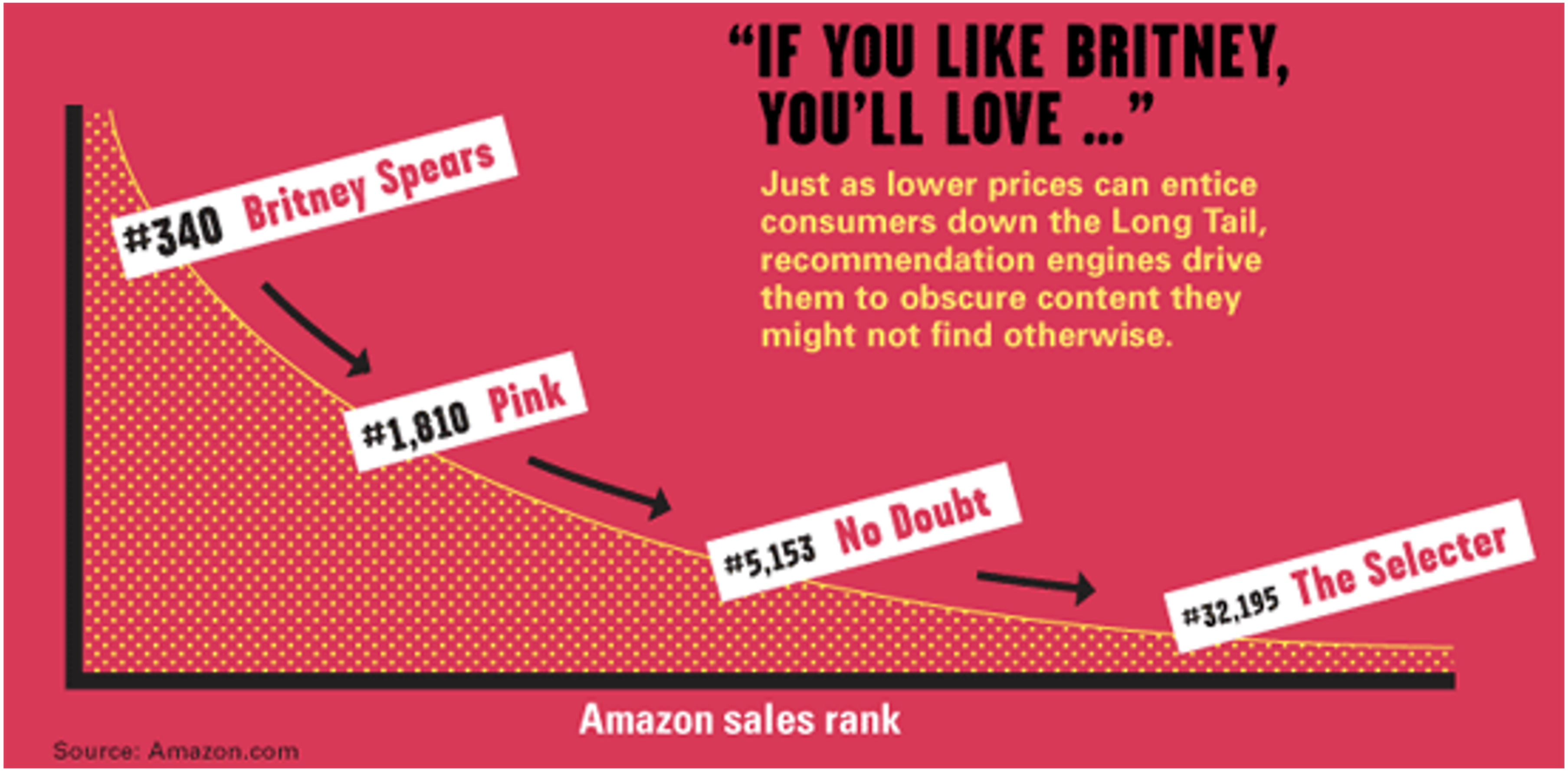


Products, web sites, blogs, news items, …

**Examples:**

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

# Long Tail



“IF YOU LIKE BRITNEY, YOU’LL LOVE ...”

Just as lower prices can entice consumers down the Long Tail, recommendation engines drive them to obscure content they might not find otherwise.

Source: Amazon.com

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

# Types of Recommendations

## 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

# Formal Model

***X*** = set of **Customers**

***S*** = set of **Items**

**Utility function** ***u***: ***X*** × ***S*** ⍰ ***R***

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

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

# 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

# Key Problems

## (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

# Gathering Ratings

## 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

# Extrapolating Utilities

**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

# Content-based

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

***Example:***

**Movie recommendations**

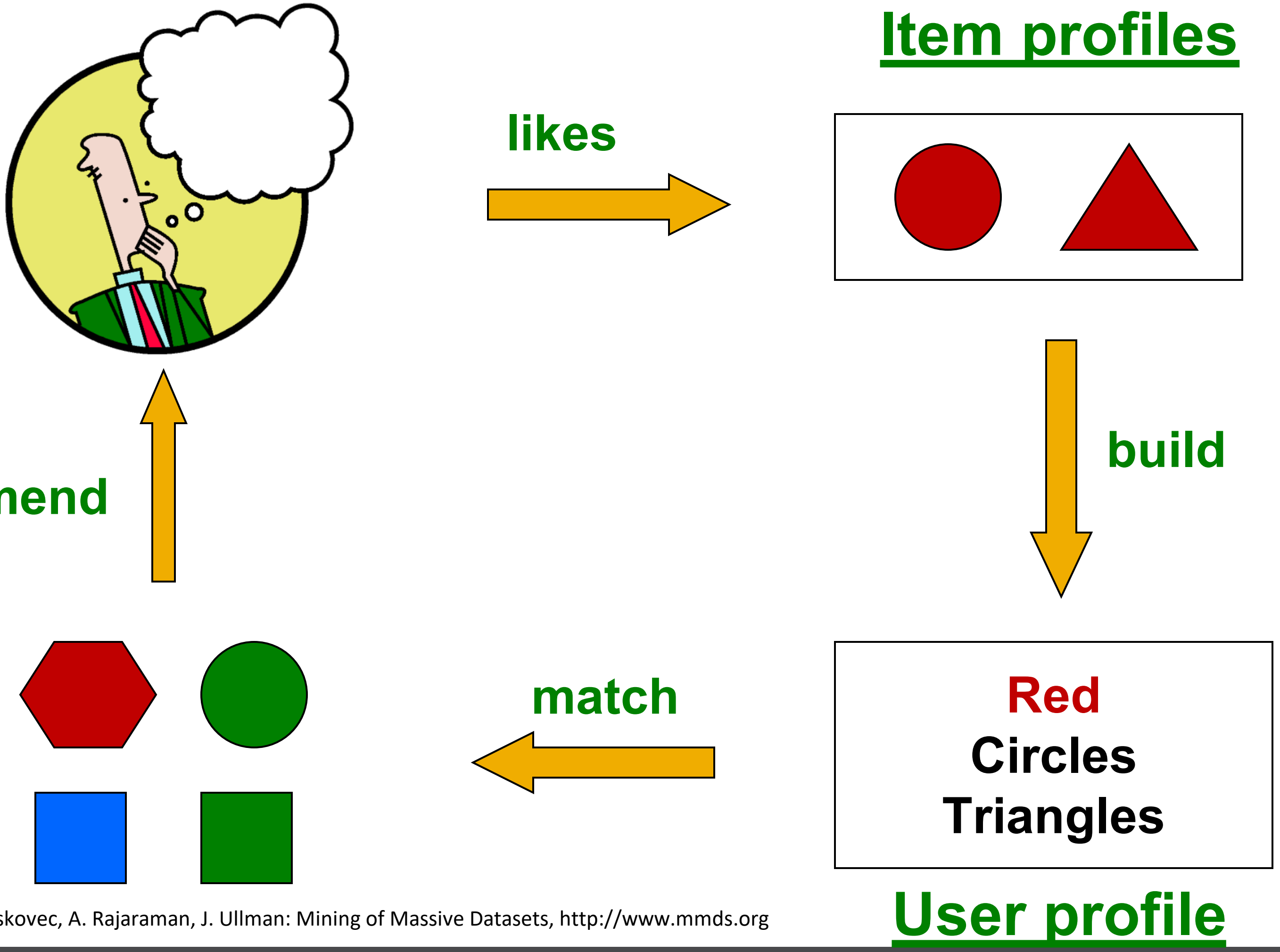
- Recommend movies with same actor(s), director, genre, …

**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



Item profiles

likes

build

Red
Circles
Triangles

User profile

match

recommend

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

# Item Profiles

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

# Users Profiles and Prediction

- **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

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

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

# Pros: Content-based

**+: 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

# Cons: Content-based

**–: 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**

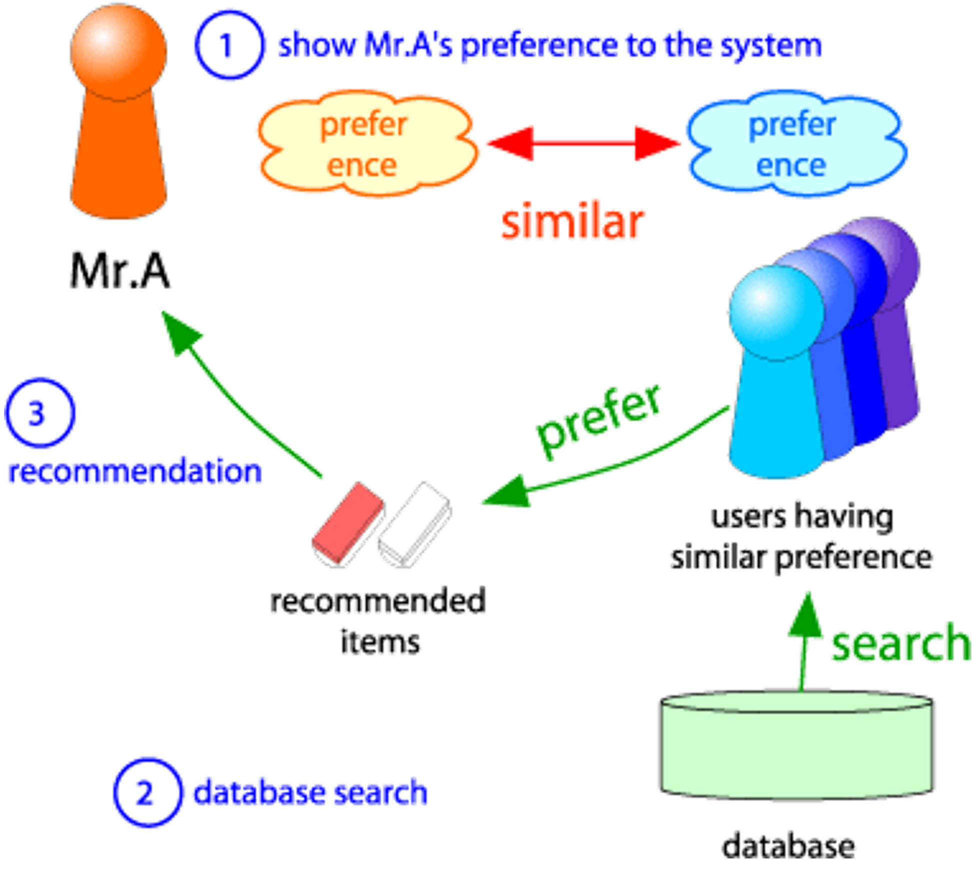
Slides adapted from J. Leskovec, A. Rajaraman, J. Ullman: Mining of Massive Datasets, http://www.mmds.org

# 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

# Pros/Cons Collab. Filtering

**+ 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:**

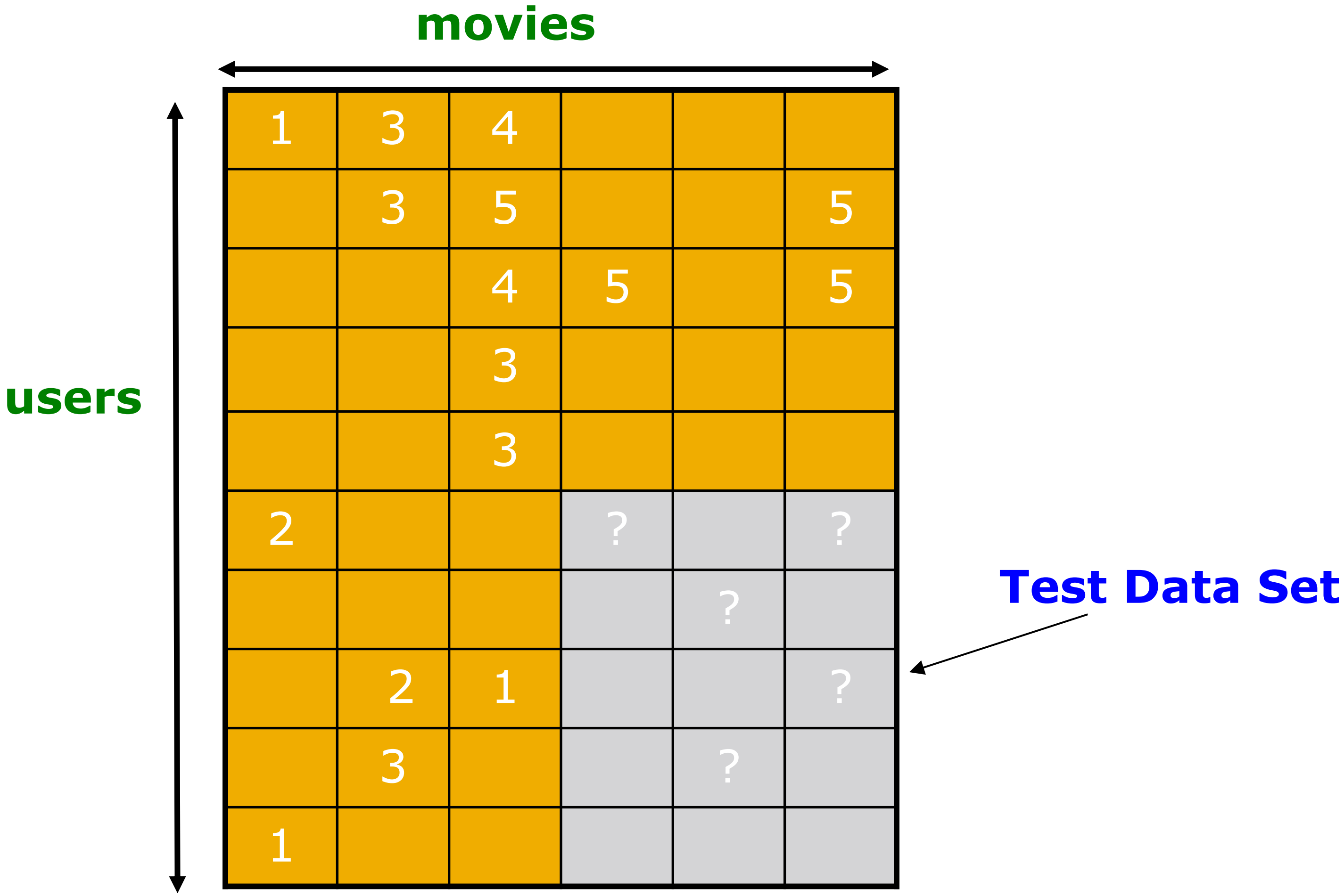
- Cannot recommend an item that has not been previously rated
- New items, Esoteric items

**- Popularity bias:**

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

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

# Offline Evaluation



| | | | | | |
|---|---|---|---|---|---|
| 1 | 3 | 4 | | | |
| | 3 | 5 | | | 5 |
| | | 4 | 5 | | 5 |
| | | 3 | | | |
| | | 3 | | | |
| 2 | | | ? | | ? |
| | | | | ? | |
| | 2 | 1 | | | ? |
| | 3 | | | ? | |
| 1 | | | | | |

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

# Evaluating Predictions

## 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

# Online Evaluation

## 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**?

—see also
**def·i·nite·ly** /ˈdefɪn
being wrong; certainly: *Max knew that he had*
*been wrong about Diana.*|"*It's not worth that much*
"*No, definitely not!*" —see OF COURSE (USAGE)
(USAGE)
**def·i·ni·tion** /ˌdefɪ̇ˈnɪʃən/ *n* **1** [C] a phrase
that says exactly what a word, phrase, or ide
*definition in a dictionary*|[+ **of**] No one has
*with a satisfactory definition of terrorism.*
**nition** if something has a particular qu
nition, it must have that quality because al
type have it: *A message that cannot be see*
*definition, not effective.* **3** [U] the degre
thing such as a picture, sound etc is
*The photograph lacks definition*
/dɪˈfɪnɪ̇tɪv/ *adj* **1** [usu

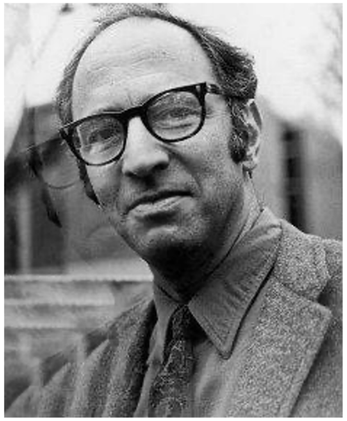
Oxford Dictionaries. 2021.

*"particular branches of study or spheres of activity or interest"*

# 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

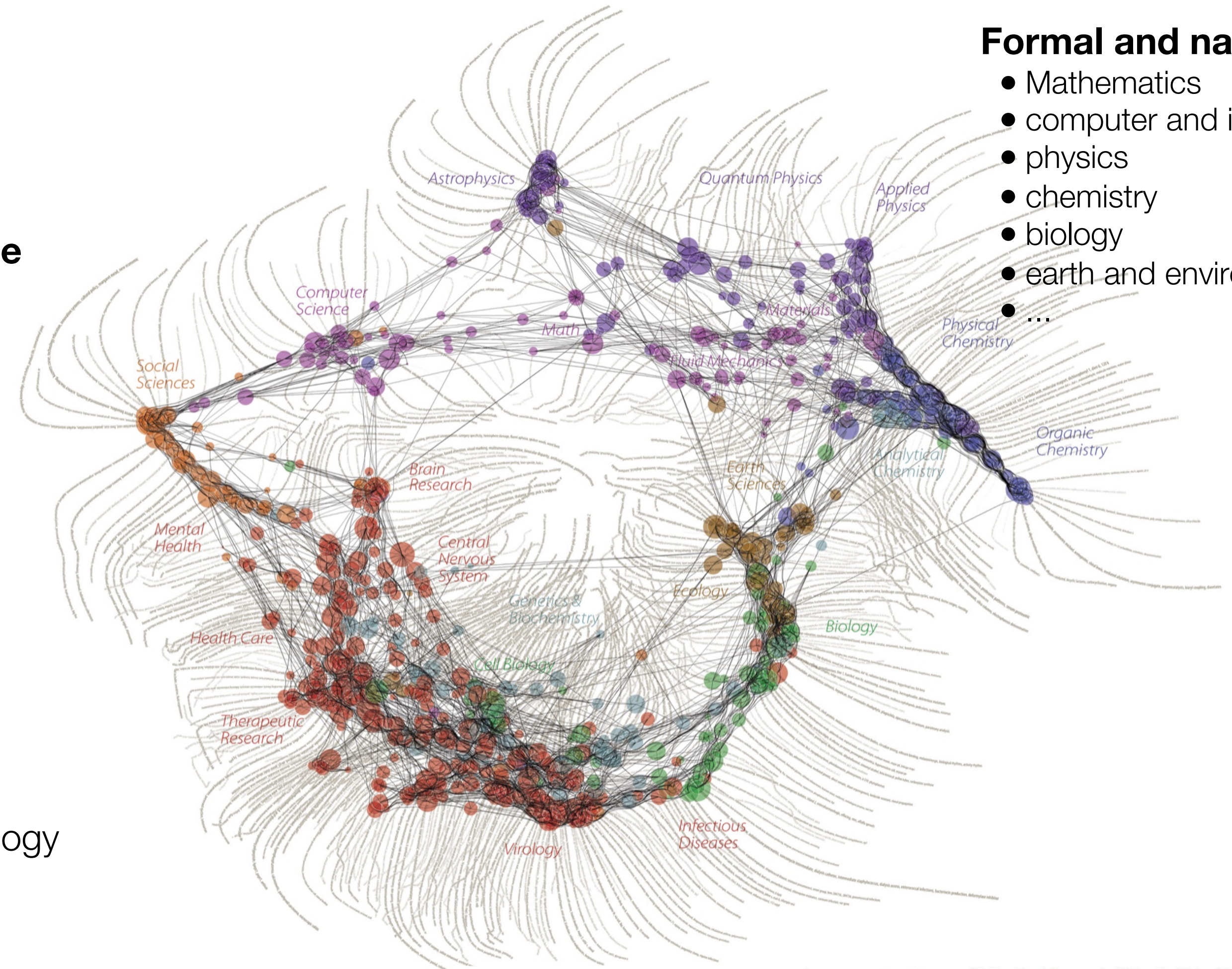
Branches of science

## Formal and natural sciences

- Mathematics
- computer and information system
- physics
- chemistry
- biology
- earth and environmental
- …

## social science

- history
- economy
- political
- …



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)

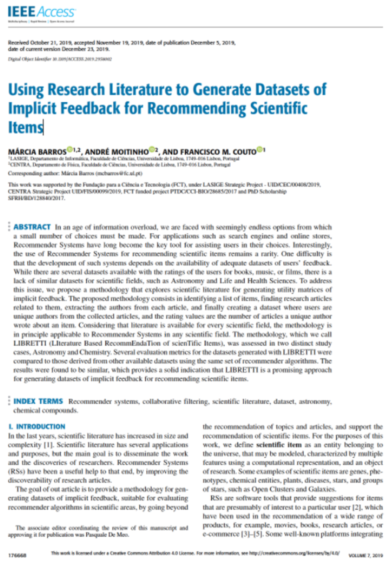
## Applied science

- health science
- health biotechnology
- …

# Scientific items

Concepts and definitions

What is mean **Scientific Items**?



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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 a small number of choices must be made. For applications such as search engines and online stores, 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 is that the development of such systems depends on the availability of adequate datasets of users' feedback. 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 issue, we propose a methodology that explores scientific literature for generating utility matrices of implicit feedback. The proposed methodology consists in identifying a list of items, finding research articles related to them, extracting the authors from each article, and finally creating a dataset where users are 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 in principle applicable to Recommender Systems in any scientific field. The methodology, which we call LIBRETTI (LIterature Based RecommEndaTion of scienTific Items), was assessed in two distinct study cases, Astronomy and Chemistry. Several evaluation metrics for the datasets generated with LIBRETTI were compared to those derived from other available datasets using the same set 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 and the discoveries of researchers. Recommender Systems (RSs) have been a useful help to that end, by improving the discoverability of research articles.

The goal of out article is to provide a methodology for generating datasets of implicit feedback, suitable for evaluating recommender algorithms in scientific areas, by going beyond the recommendation of topics and articles, and support the recommendation of scientific items. For the purposes of this work, we define **scientific item** as an entity belonging to the universe, that may be modeled, characterized by multiple features using a computational representation, and an object of research. Some examples of scientific items are genes, phenotypes, chemical entities, plants, diseases, stars, and groups of stars, such as Open Clusters and Galaxies.

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

The associate editor coordinating the review of this manuscript and approving it for publication was Pasquale De Meo.

"(...) 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}”

{ collaborative OR content-based } AND filtering }

# Literature review

Search process

### include

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

### exclude

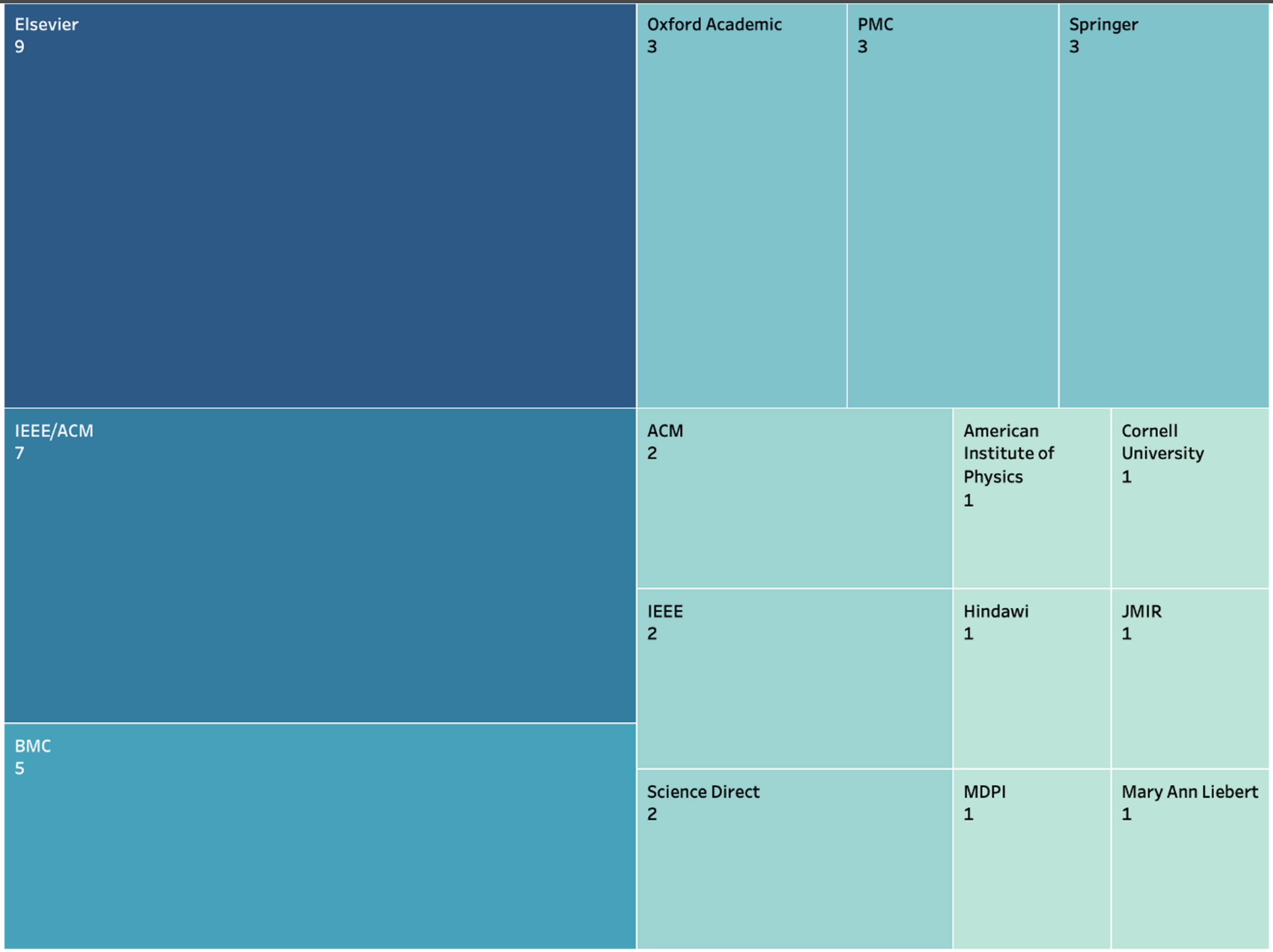
1. manuscripts written in other language than english
2. technical reports, master and PhD dissertation
3. surveys

### criteria of selection

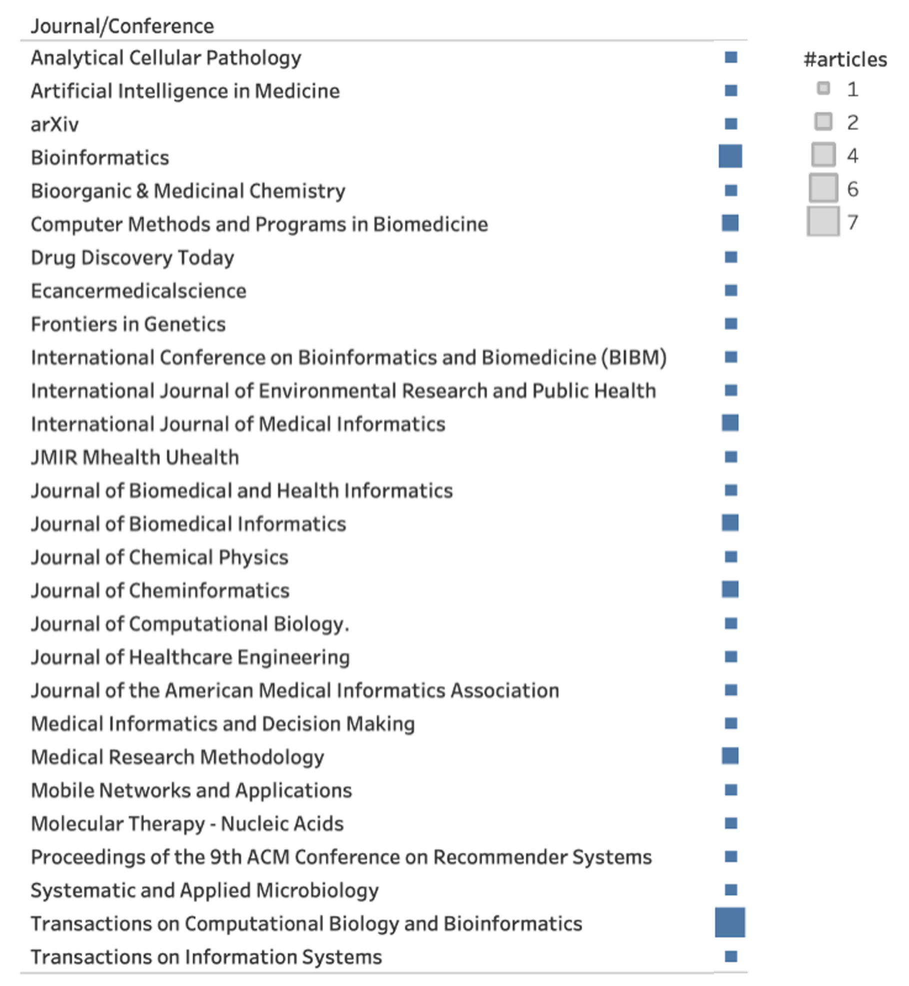
1. clearly stated objectives, results and findings on the domain of knowledge
2. well-presented and justified arguments
3. well-referenced with a minimum of 10 sources

# Trends of a Glance: publisher

#articles



# Journal and conference



Journal/Conference

Analytical Cellular Pathology

Artificial Intelligence in Medicine

arXiv

Bioinformatics

Bioorganic & Medicinal Chemistry

Computer Methods and Programs in Biomedicine

Drug Discovery Today

Ecancermedicalscience

Frontiers in Genetics

International Conference on Bioinformatics and Biomedicine (BIBM)

International Journal of Environmental Research and Public Health

International Journal of Medical Informatics

JMIR Mhealth Uhealth

Journal of Biomedical and Health Informatics

Journal of Biomedical Informatics

Journal of Chemical Physics

Journal of Cheminformatics

Journal of Computational Biology.

Journal of Healthcare Engineering

Journal of the American Medical Informatics Association

Medical Informatics and Decision Making

Medical Research Methodology

Mobile Networks and Applications

Molecular Therapy - Nucleic Acids

Proceedings of the 9th ACM Conference on Recommender Systems

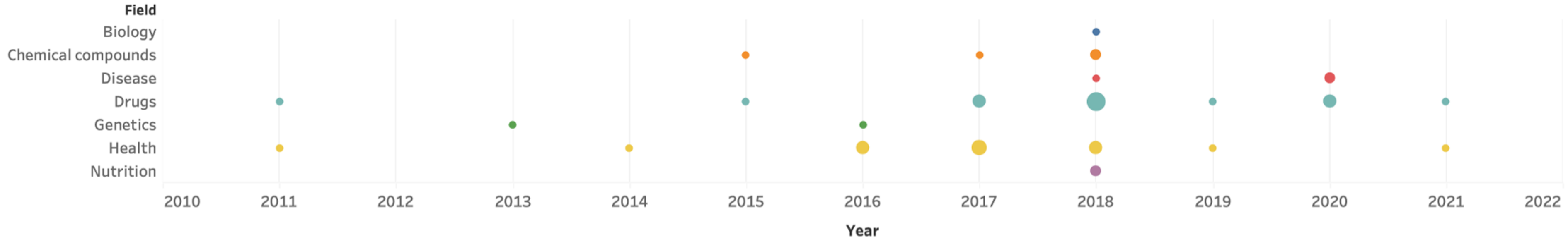
Systematic and Applied Microbiology

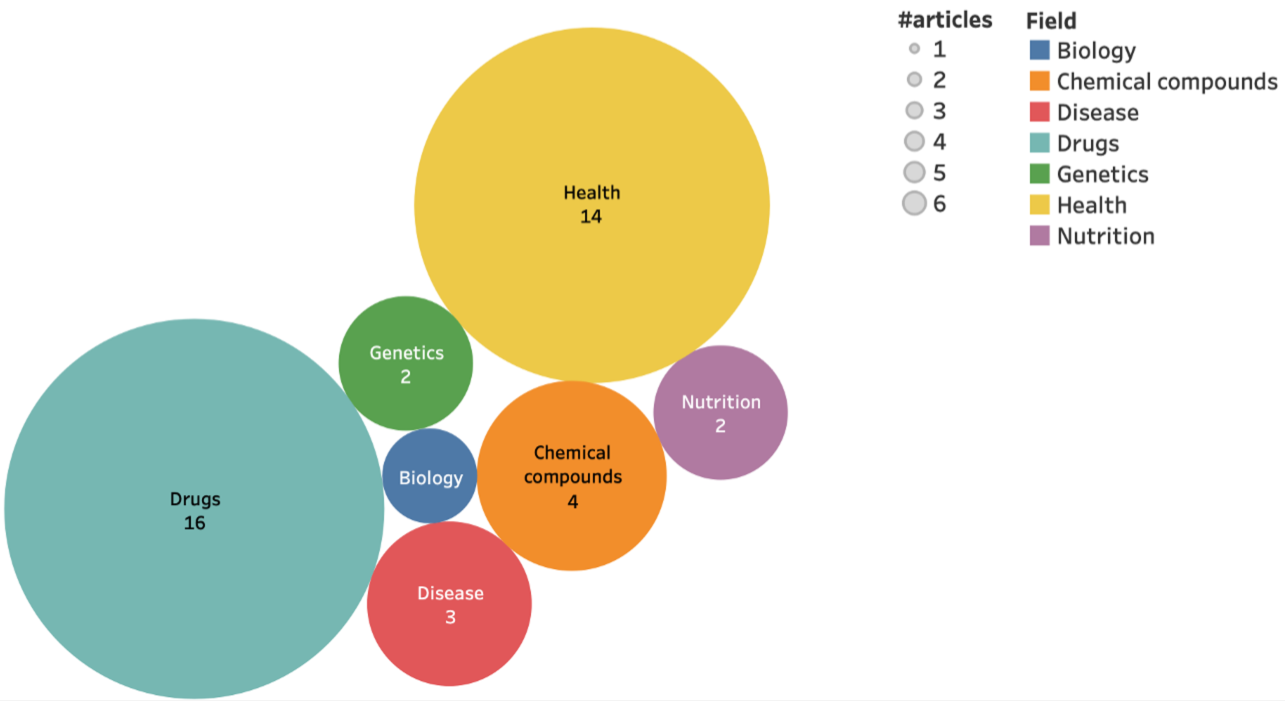
Transactions on Computational Biology and Bioinformatics

Transactions on Information Systems

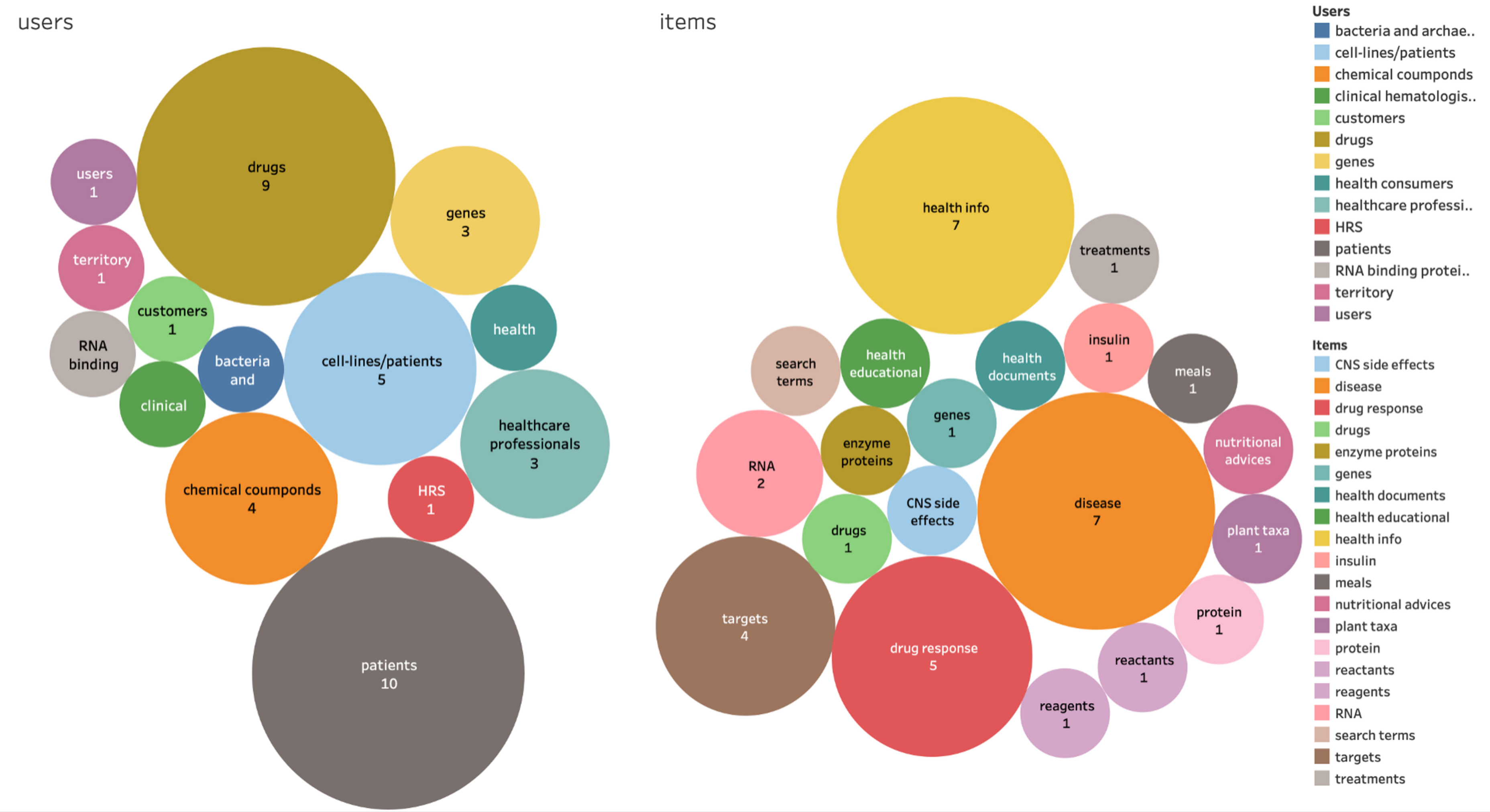
# Scientific fields

#articles

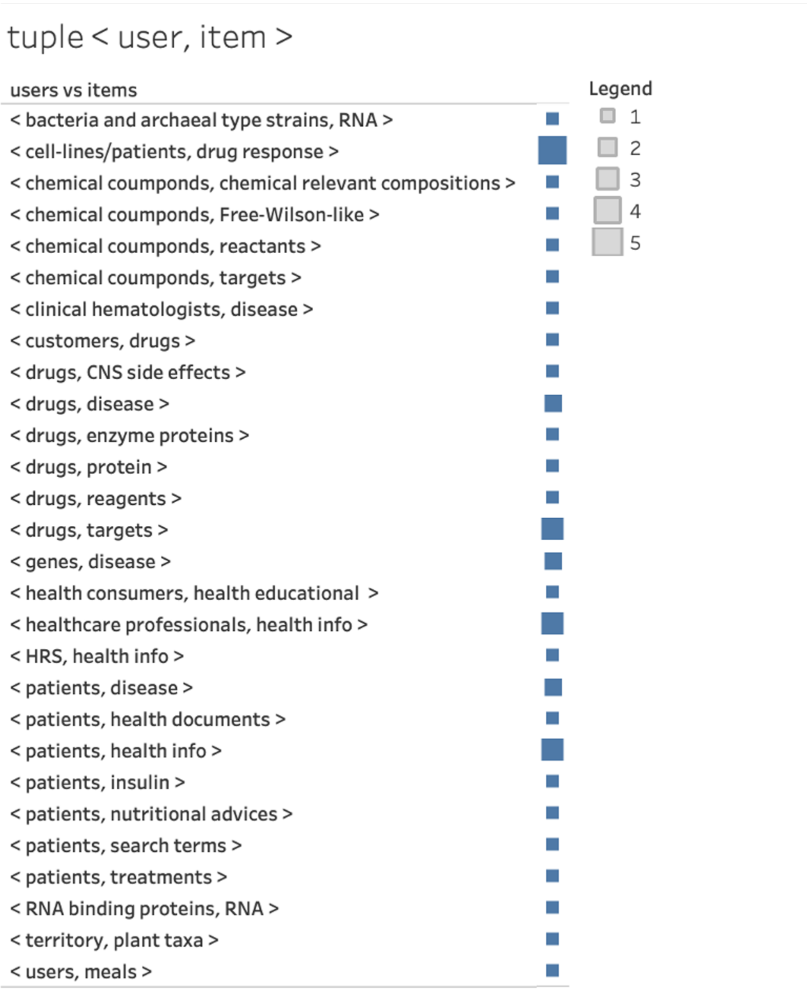




# Matrix Factorization



# tuple: < user, item >



tuple < user, item >

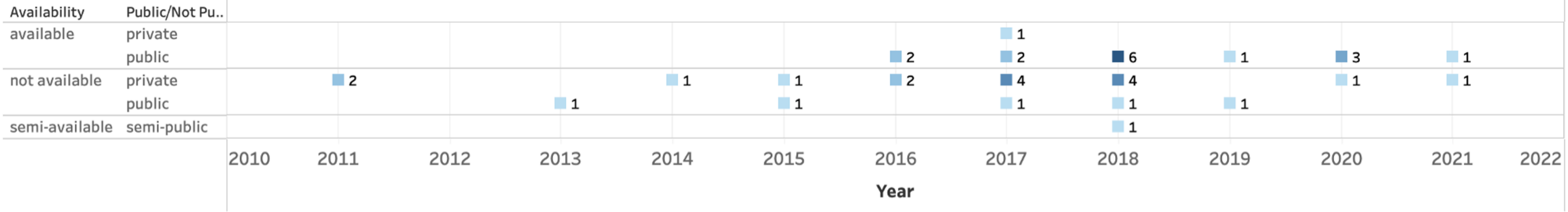
users vs items

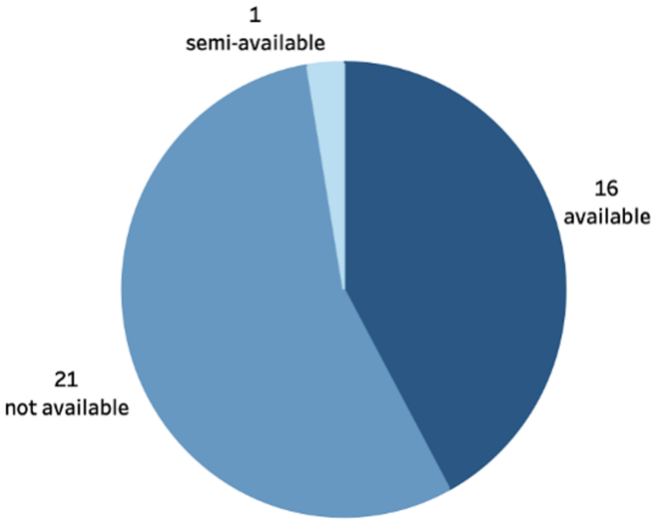
< bacteria and archaeal type strains, RNA >
< cell-lines/patients, drug response >
< chemical coumponds, chemical relevant compositions >
< chemical coumponds, Free-Wilson-like >
< chemical coumponds, reactants >
< chemical coumponds, targets >
< clinical hematologists, disease >
< customers, drugs >
< drugs, CNS side effects >
< drugs, disease >
< drugs, enzyme proteins >
< drugs, protein >
< drugs, reagents >
< drugs, targets >
< genes, disease >
< health consumers, health educational >
< healthcare professionals, health info >
< HRS, health info >
< patients, disease >
< patients, health documents >
< patients, health info >
< patients, insulin >
< patients, nutritional advices >
< patients, search terms >
< patients, treatments >
< RNA binding proteins, RNA >
< territory, plant taxa >
< users, meals >

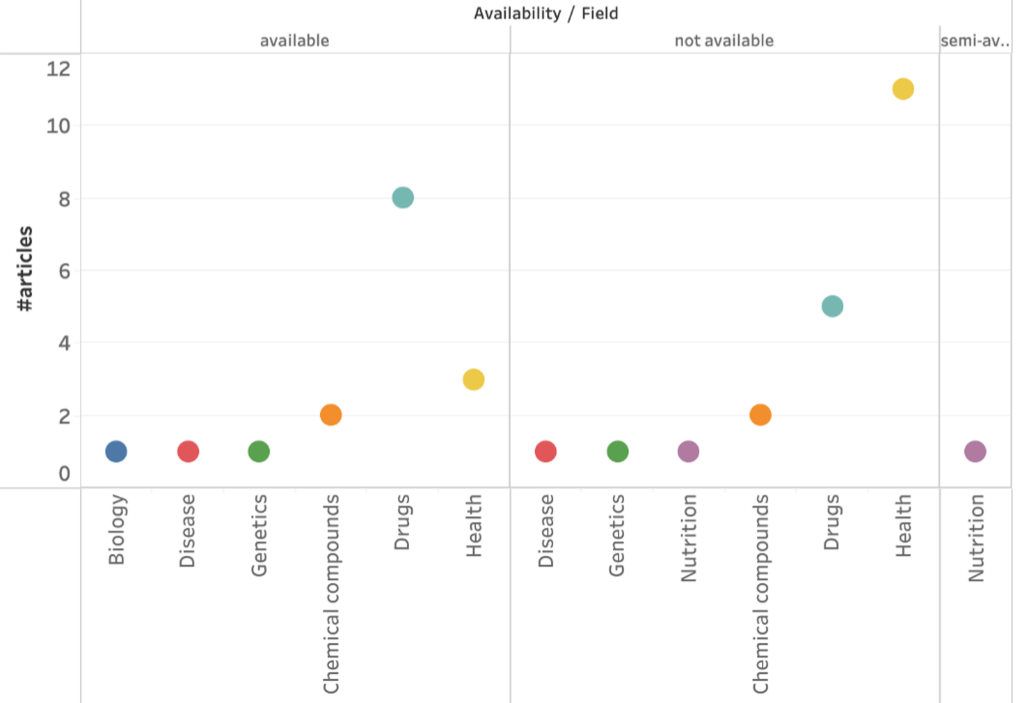
Legend

- 1
- 2
- 3
- 4
- 5

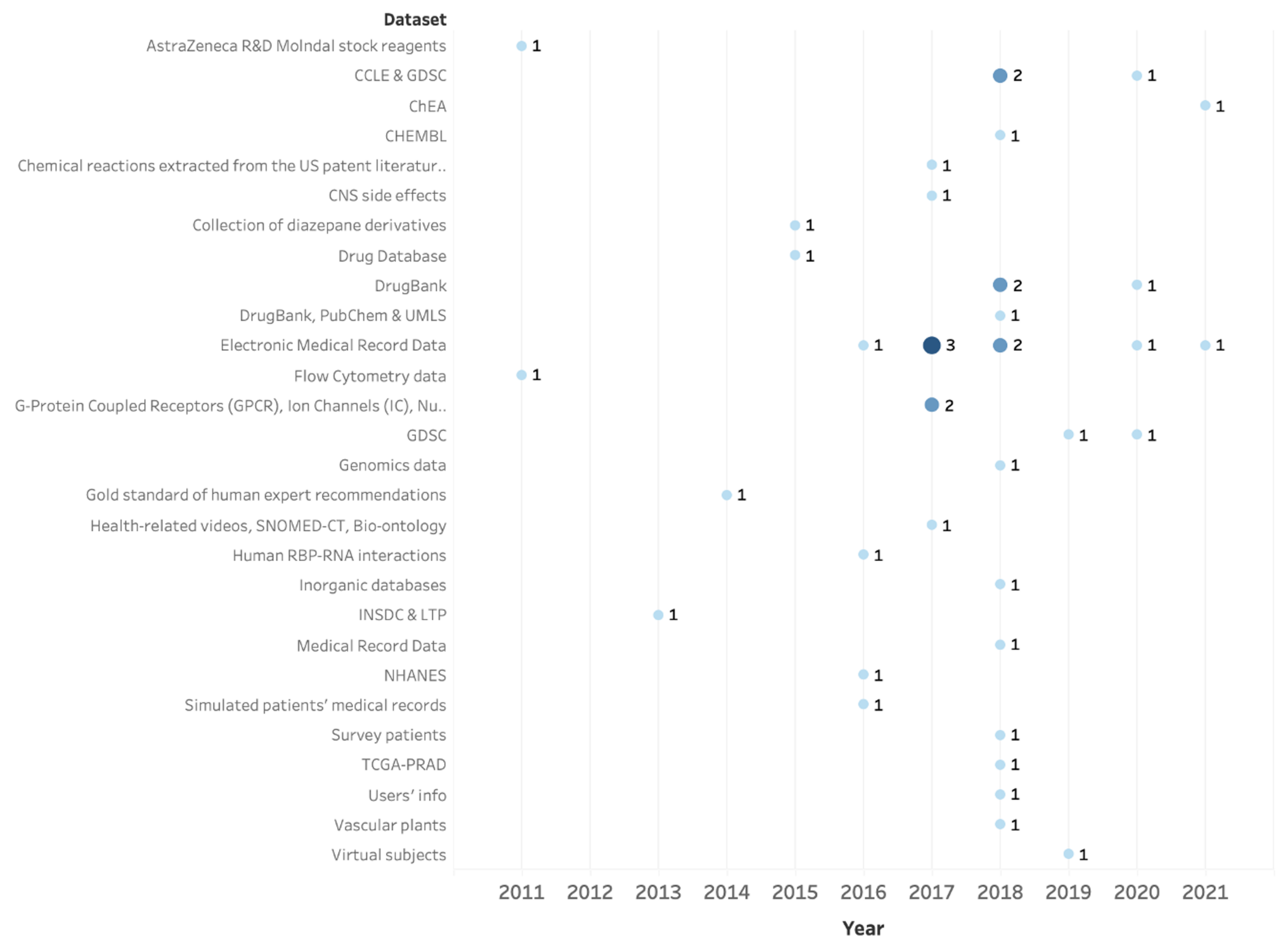
# Availability of the dataset







# Source of the dataset



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

**Pedro Ruas**

# Scientific/biomedical knowledge

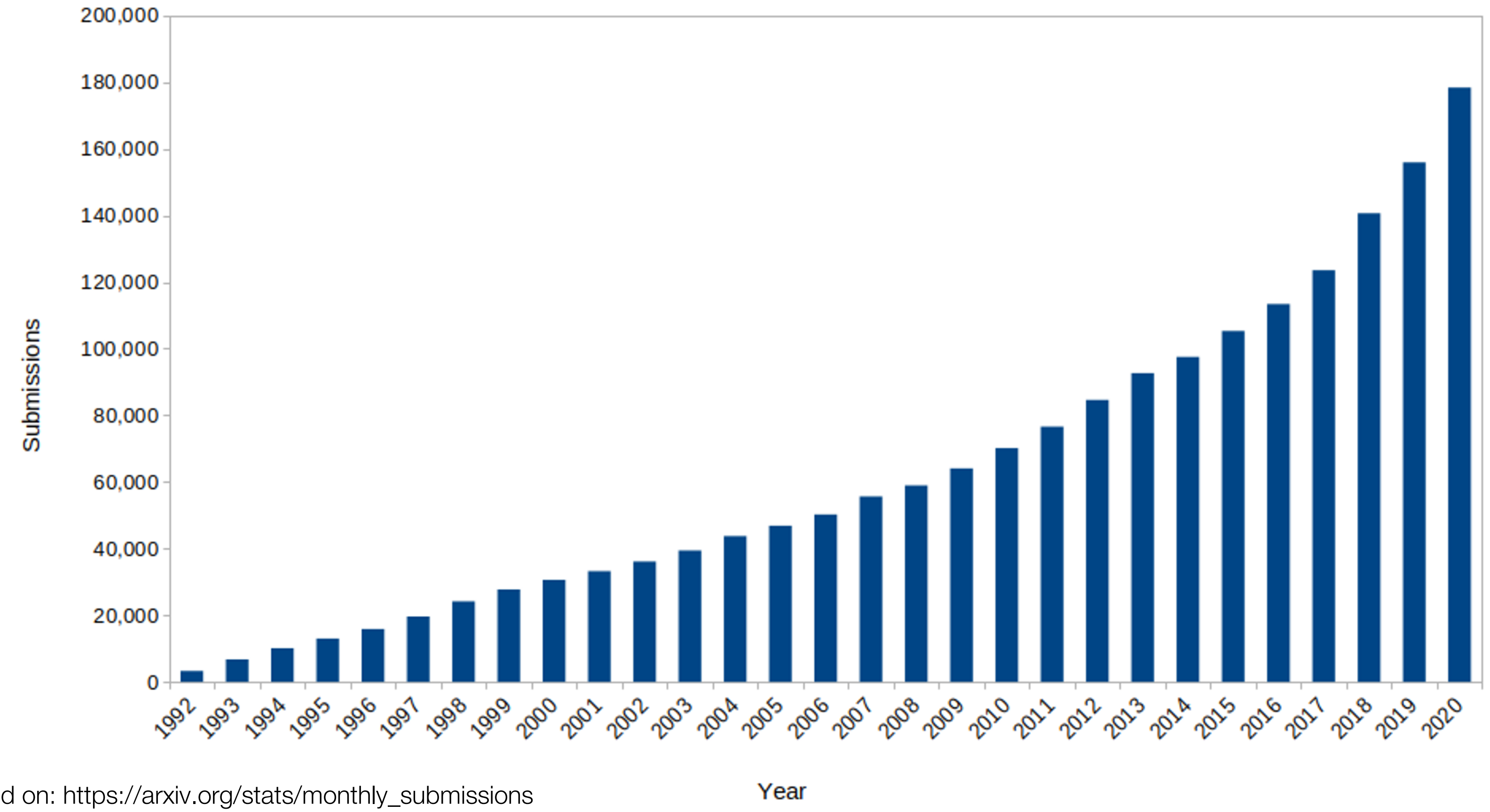
Described in text in:

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

# Scientific/biomedical knowledge

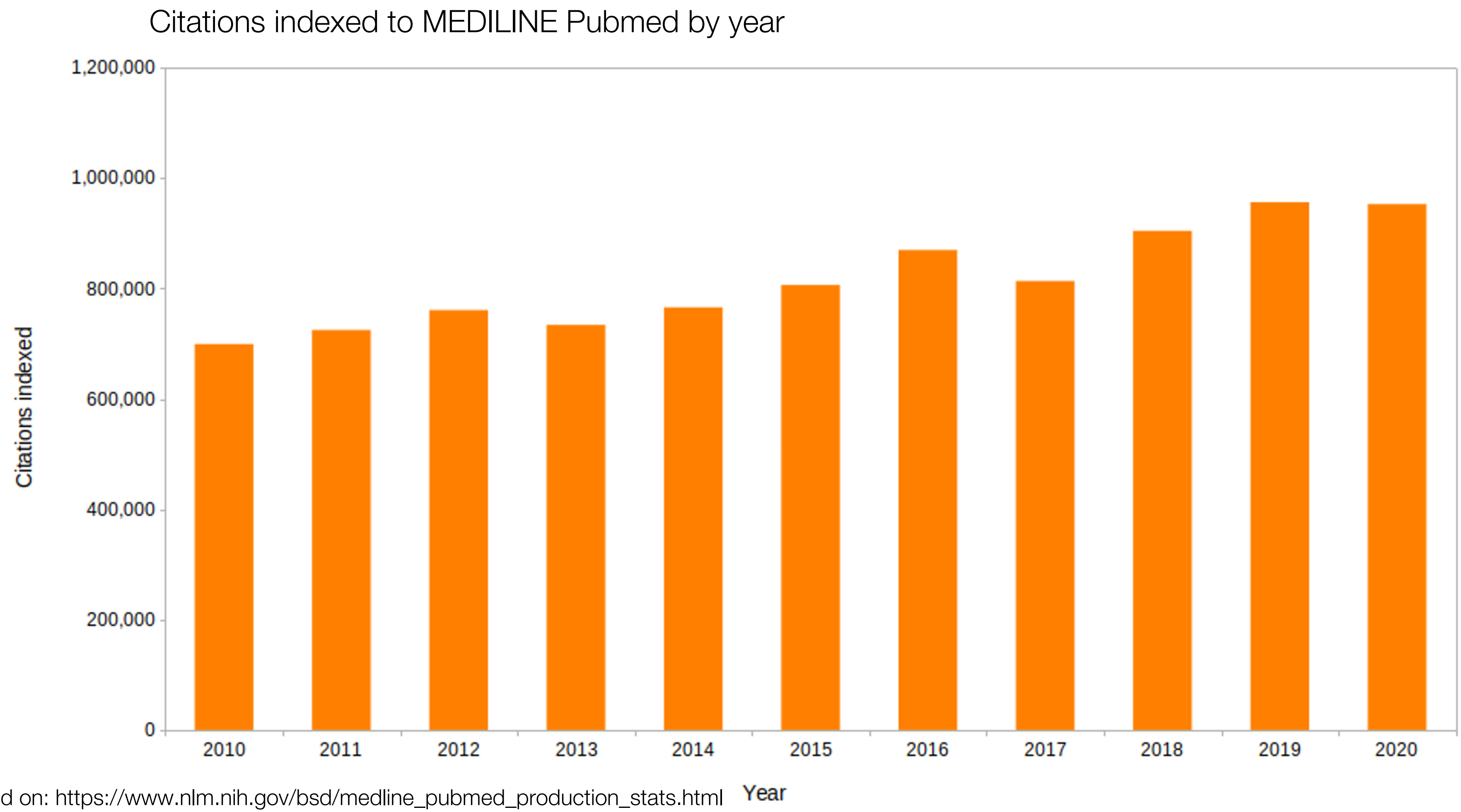
LASIGE driven by excellence

New submissions to arXiv by year



Based on: https://arxiv.org/stats/monthly_submissions

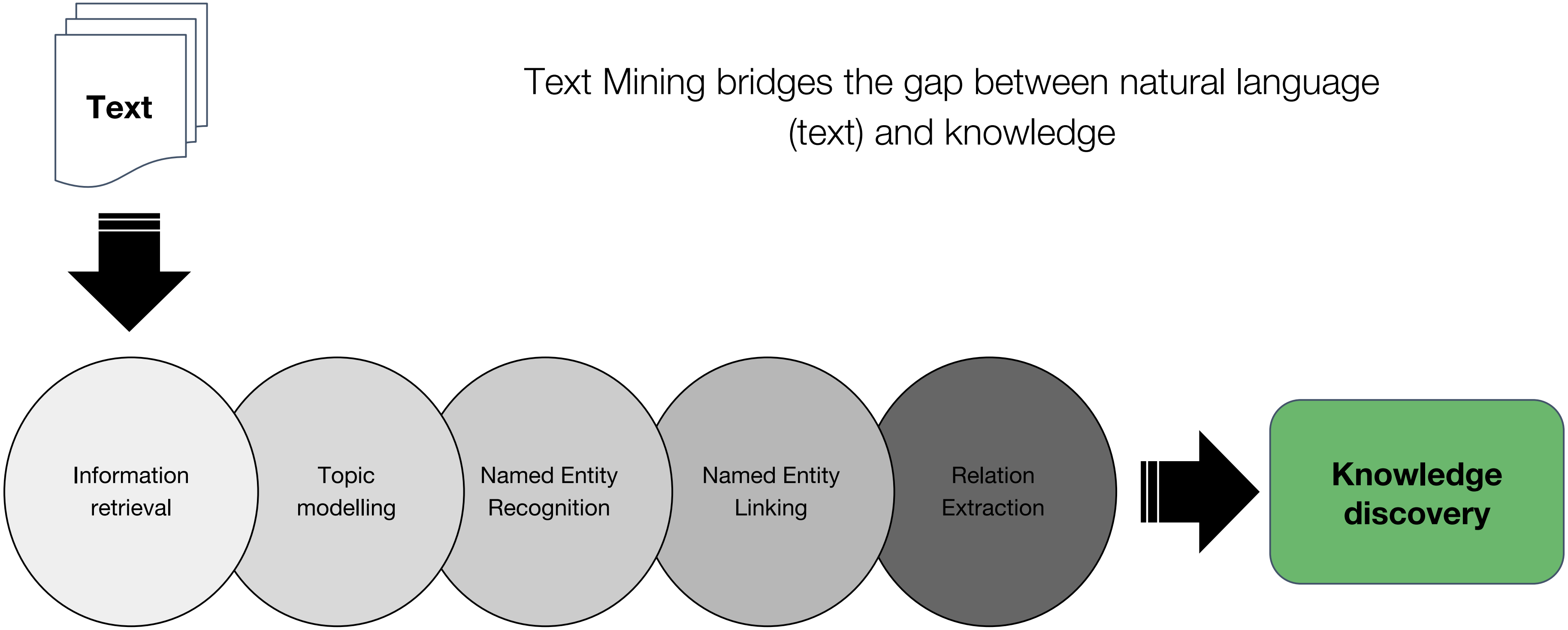
# Scientific/biomedical knowledge



Based on: https://www.nlm.nih.gov/bsd/medline_pubmed_production_stats.html

# Text Mining

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



Text

Information retrieval

Topic modelling

Named Entity Recognition

Named Entity Linking

Relation Extraction

**Knowledge discovery**

**Text Mining tasks**

# 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.»* [1]

Another definition (2018):

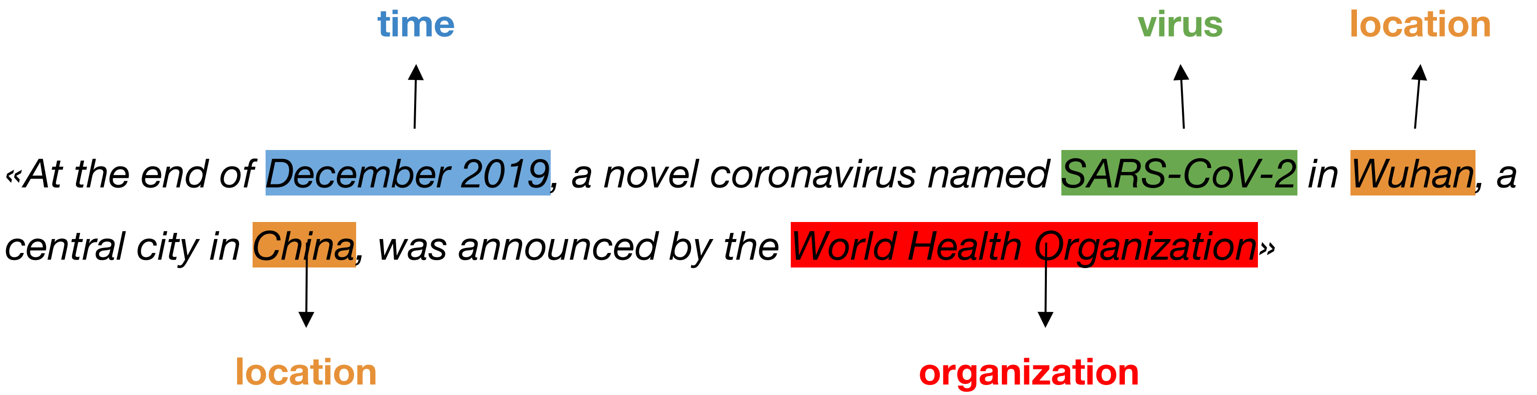
> *«Named Entity Recognition and Classification, an important sub-task of Information Extraction, points to* ***identify*** *and* ***classify*** *members of rigid designators from data suited to different types of named entities such as organizations, persons, locations, etc.»* [2]

[1] 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.
[2] 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

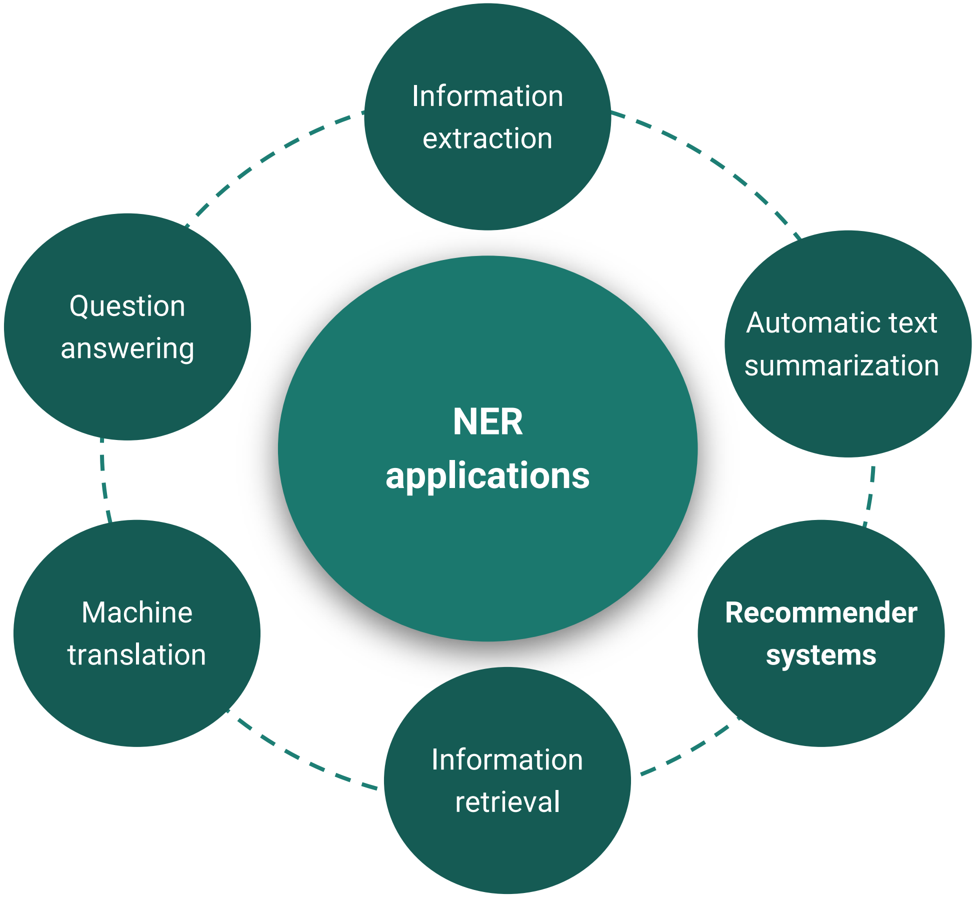


*«At the end of December 2019, a novel coronavirus named SARS-CoV-2 in Wuhan, a central city in China, was announced by the World Health Organization»*

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

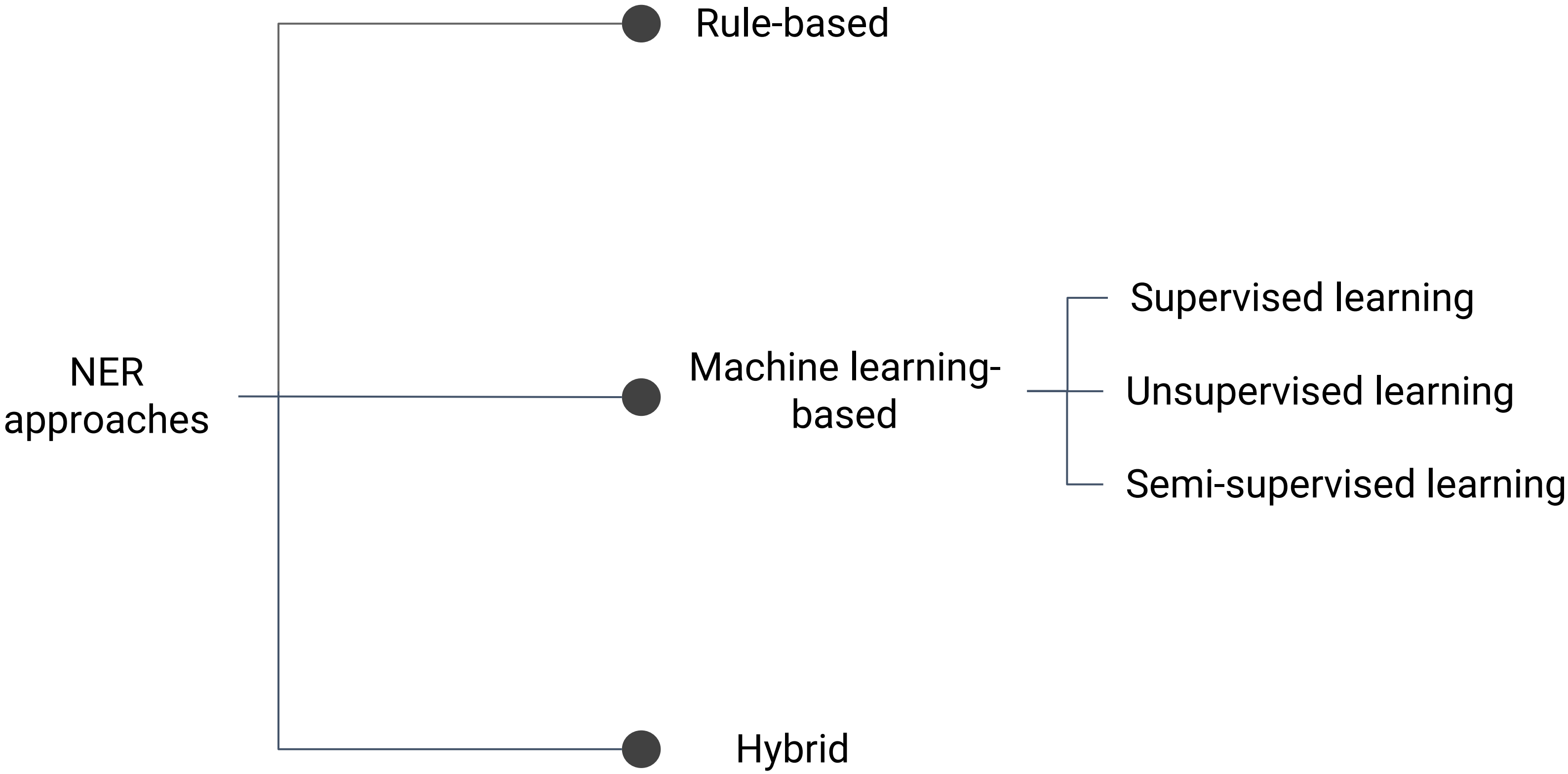
# Named Entity Recognition

## Applications



# Named Entity Recognition

Types of systems

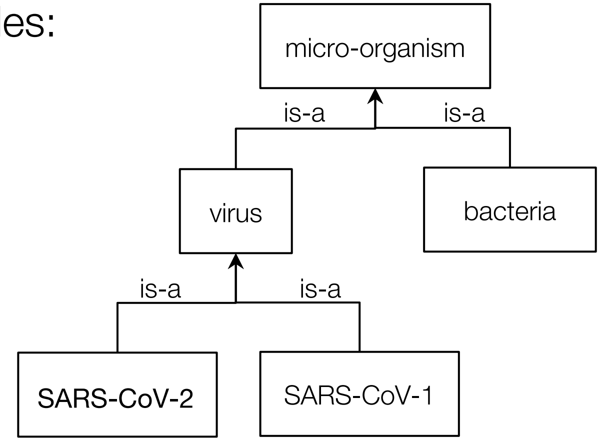


Based on A. Goyal, V. Gupta, and M. Kumar, "Recent Named Entity Recognition and Classification techniques: A systematic review," *Comput. Sci. Rev.*, vol. 29, pp. 21–43, 2018, doi: 10.1016/j.cosrev.2018.06.001.

# Knowledge Bases

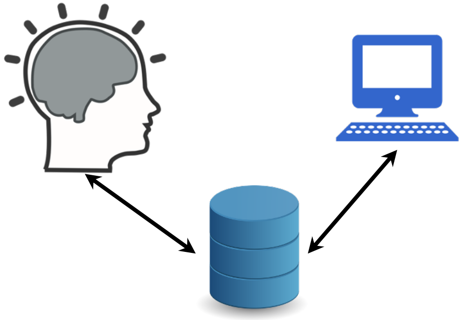
Formal representation of the reality or a part of it, which includes:

- ➔ 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

WIKIPEDIA

DBpedia

## In the biomedical domain

GENEONTOLOGY
Unifying Biology

DISEASE ONTOLOGY

ChEBI

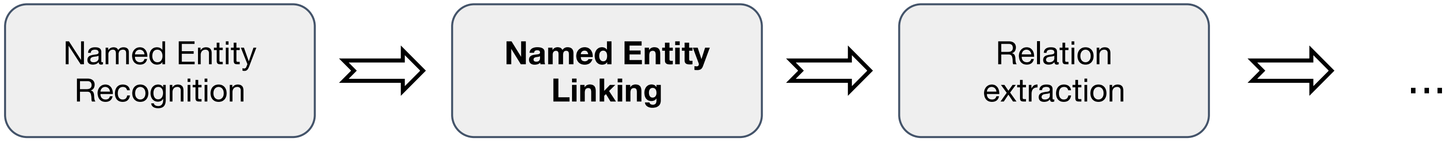
MeSH

# 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.»* [1]

Text Mining Pipeline



[1] 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)

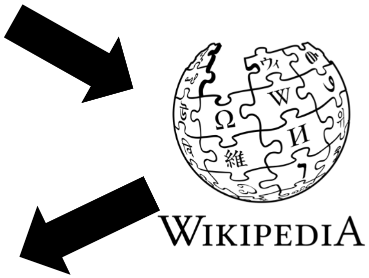
Definition

**Example**

time | virus | location

*«At the end of December 2019, a novel coronavirus named SARS-CoV-2 in Wuhan, a central city in China, was announced by the World Health Organization»*

location | organization

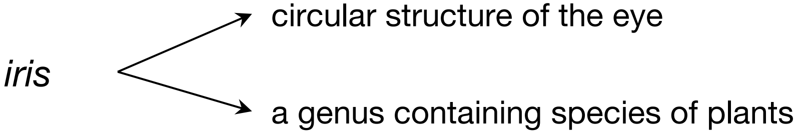


| **Entity** | **Category** | **Begin** | **End** | **URL** |
|---|---|---|---|---|
| “December 2019” | time | 13 | 26 | https://en.wikipedia.org/wiki/2019#December |
| “SARS-CoV-2” | virus | 54 | 64 | https://en.wikipedia.org/wiki/Severe_acute_respiratory_syndrome_coronavirus_2 |
| “Wuhan” | location | 68 | 73 | https://en.wikipedia.org/wiki/Wuhan |
| “China” | location | 93 | 98 | https://en.wikipedia.org/wiki/China |
| “World Health Organization” | organization | 121 | 146 | https://en.wikipedia.org/wiki/World_Health_Organization |

# Named Entity Linking (NEL)

## Challenges

- **Ambiguity**

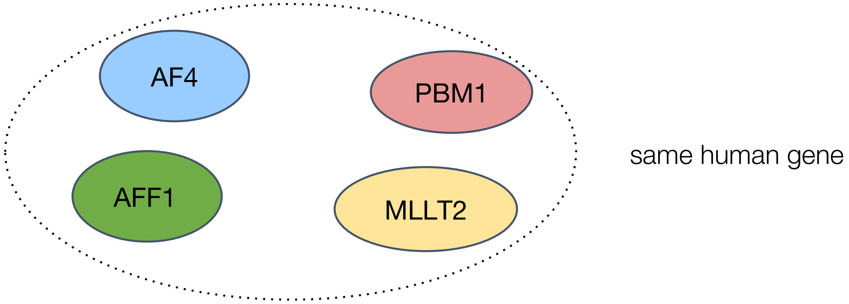


*iris*

circular structure of the eye

a genus containing species of plants

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



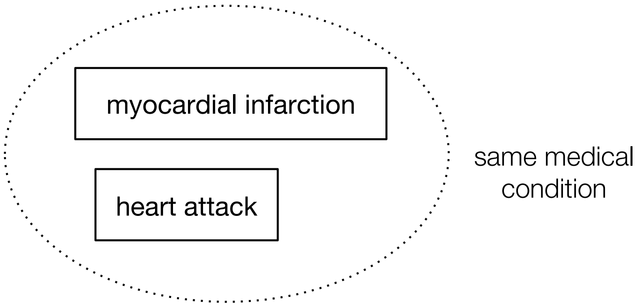
AF4

PBM1

AFF1

MLLT2

same human gene



myocardial infarction

heart attack

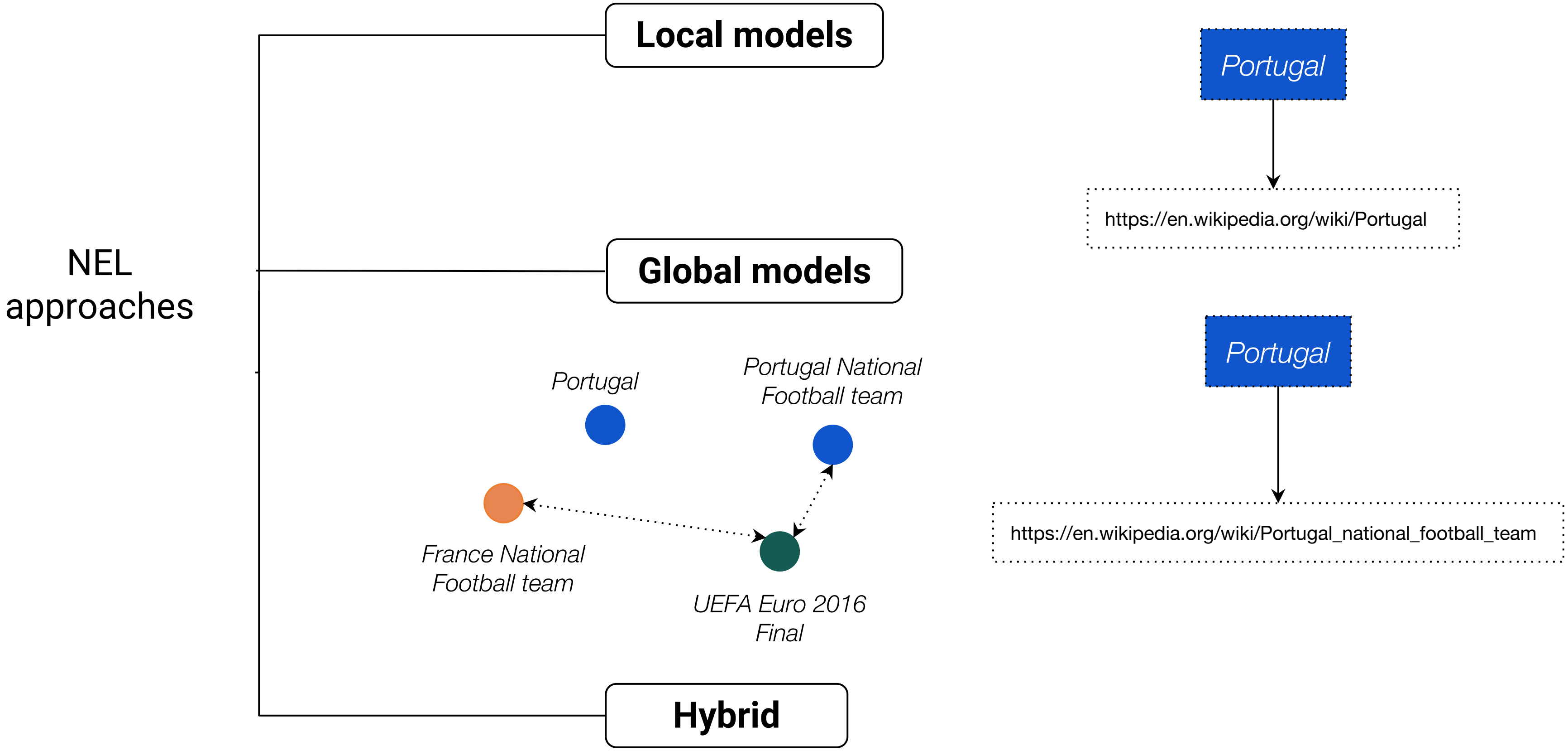
same medical condition

- **Incomplete ontologies/KBs**

# Named Entity Linking (NEL)

## Types of systems

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



NEL approaches

**Local models**

*Portugal*

https://en.wikipedia.org/wiki/Portugal

**Global models**

*Portugal*

*Portugal National Football team*

*France National Football team*

*UEFA Euro 2016 Final*

*Portugal*

https://en.wikipedia.org/wiki/Portugal_national_football_team

**Hybrid**

# 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.**»* [1]

[1] Y. Betancourt and S. Ilarri, "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.
4. P. Basile and C. Musto, "Aggregation strategies for linked open data-enabled recommender systems," in *2014 Europ. Semantic Web Conf. (Linked Open Data-enabled Recomm. Syst. Challenge)*, 2014, pp. 1–5, [Online]. Available: http://2014.eswc-conferences.org/sites/default/files/eswc2014-challenges_rs_submission_16.pdf.

# NER + NEL + Recommender systems

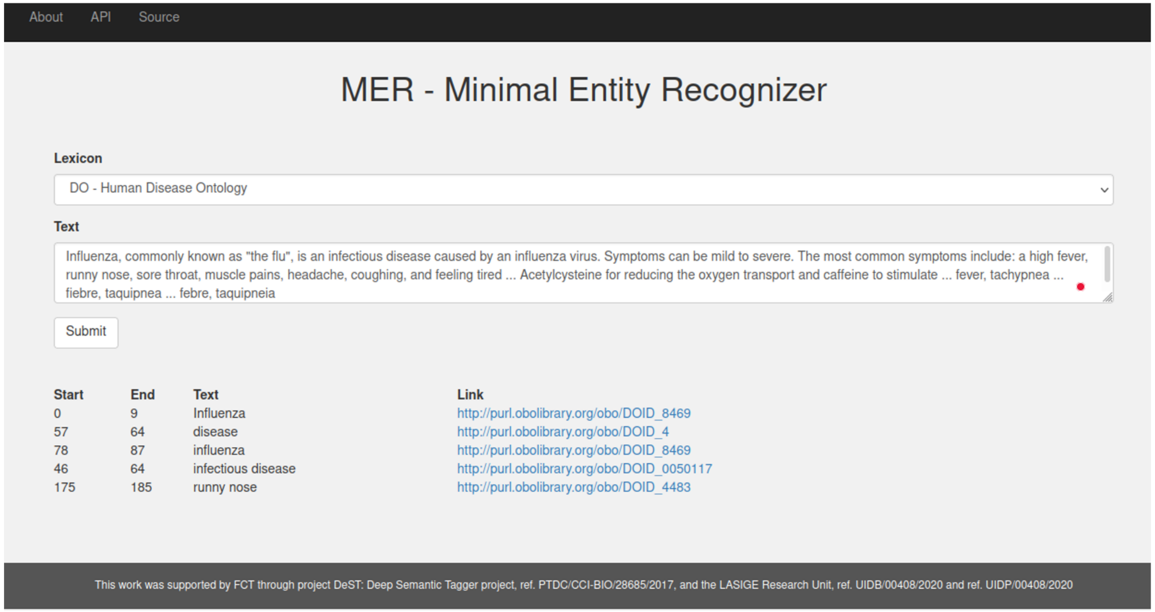
| Ref | Field | RS type | Role of NER/NEL | NER/NEL Tool | Ontologies |
|---|---|---|---|---|---|
| 5 | Agro-business web pages | Collaborative-filtering | To extract entities from web pages to enrich the dataset | - | - |
| 6 | Agro-business web pages, movies | Collaborative-filtering | To extract entities 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 |

5. M. A. Domingues *et al.*, "Applying multi-view based metadata in personalized ranking for recommender systems," in *Proceedings of the ACM Symposium on Applied Computing*, 2015, vol. 13-17-Apri, pp. 1105-1107, doi: 10.1145/2695664.2695955.
6. M. G. Manzato *et al.*, "Mining unstructured content for recommender systems: An ensemble approach," *Inf. Retr. J.*, vol. 19, no. 4, pp. 378–415, 2016, doi: 10.1007/s10791-016-9280-8.
7. T. Eftimov, B. K. Seljak, and P. Korošec, *A rule-based named-entity recognition method for knowledge extraction of evidence-based dietary recommendations*, vol. 12, no. 6. 2017.
8. C. Limongelli, M. Lombardi, A. Marani, and D. Taibi, "Enrichment of the Dataset of Joint Educational Entities with the Web of Data," in *Proceedings - IEEE 17th International Conference on Advanced Learning Technologies, ICALT 2017*, 2017, pp. 528–529, doi: 10.1109/ICALT.2017.13.
9. A. Iovine, F. Narducci, and G. Semeraro, "Conversational Recommender Systems and natural language:: A study through the ConveRSE framework," *Decis. Support Syst.*, vol. 131, no. June 2019, 2020, doi: 10.1016/j.dss.2020.113250.

# MER

Minimal Named Entity Recognizer

- 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, taquipneia

| Start | End | Text | Link |
|---|---|---|---|
| 0 | 9 | Influenza | http://purl.obolibrary.org/obo/DOID_8469 |
| 57 | 64 | disease | http://purl.obolibrary.org/obo/DOID_4 |
| 78 | 87 | influenza | http://purl.obolibrary.org/obo/DOID_8469 |
| 46 | 64 | infectious disease | http://purl.obolibrary.org/obo/DOID_0050117 |
| 175 | 185 | runny nose | http://purl.obolibrary.org/obo/DOID_4483 |

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

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.

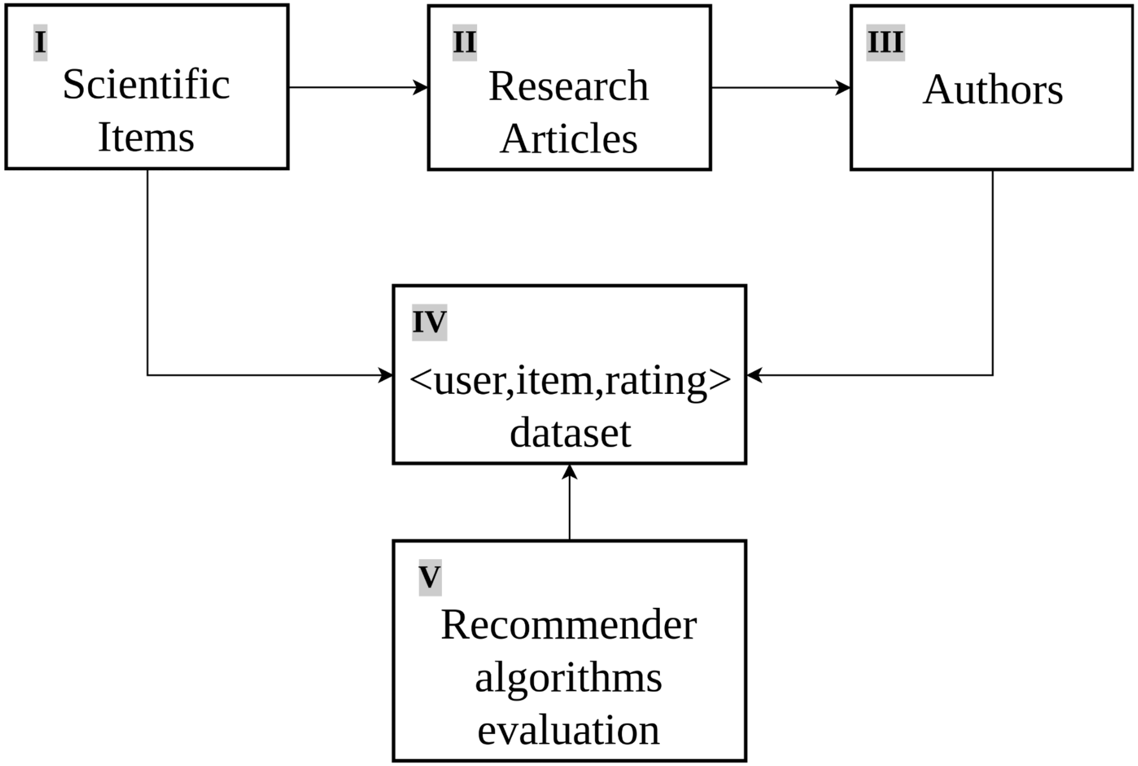
# LIterature Based RecommEndaTion of scienTific Items (LIBRETTI)

**Márcia Barros**

# LIBRETTI

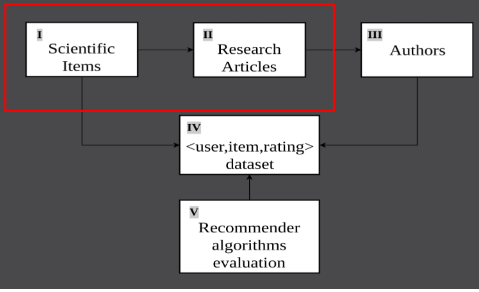
general pipeline

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



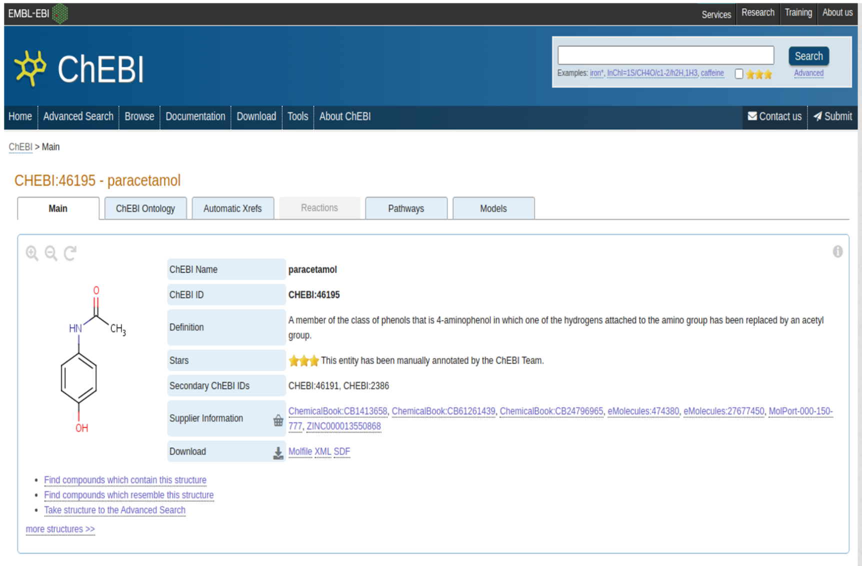
# LIBRETTI

knowledge base


I Scientific Items
II Research Articles
III Authors
IV <user,item,rating> dataset
V Recommender algorithms evaluation

LASIGE driven by excellence

knowledge base with information about research articles mentioning the entities



Examples: iron*, InChI=1S/CH4O/c1-2/h2H,1H3, caffeine □ ★★★

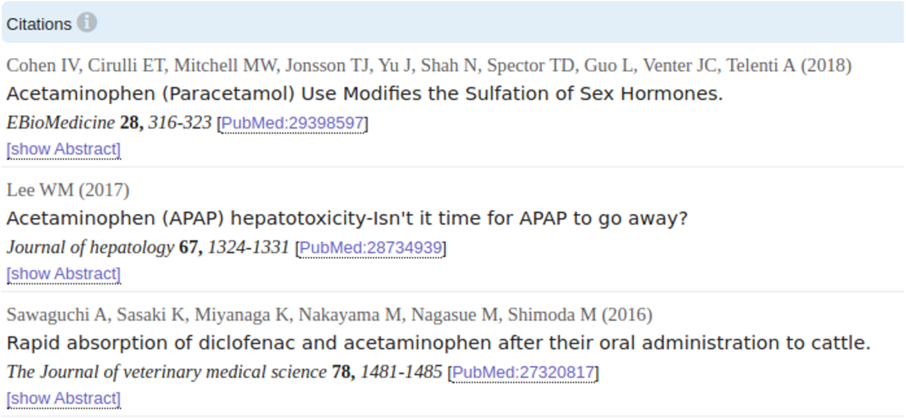
ChEBI > Main

CHEBI:46195 - 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]

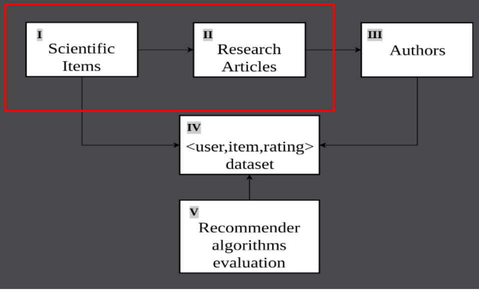
Sawaguchi A, Sasaki K, Miyanaga K, Nakayama M, Nagasue M, Shimoda M (2016)
Rapid absorption of diclofenac and acetaminophen after their oral administration to cattle.
*The Journal of veterinary medical science* **78,** *1481-1485* [PubMed:27320817]
[show Abstract]

Ciências ULisboa

FCT Fundação para a Ciência e a Tecnologia

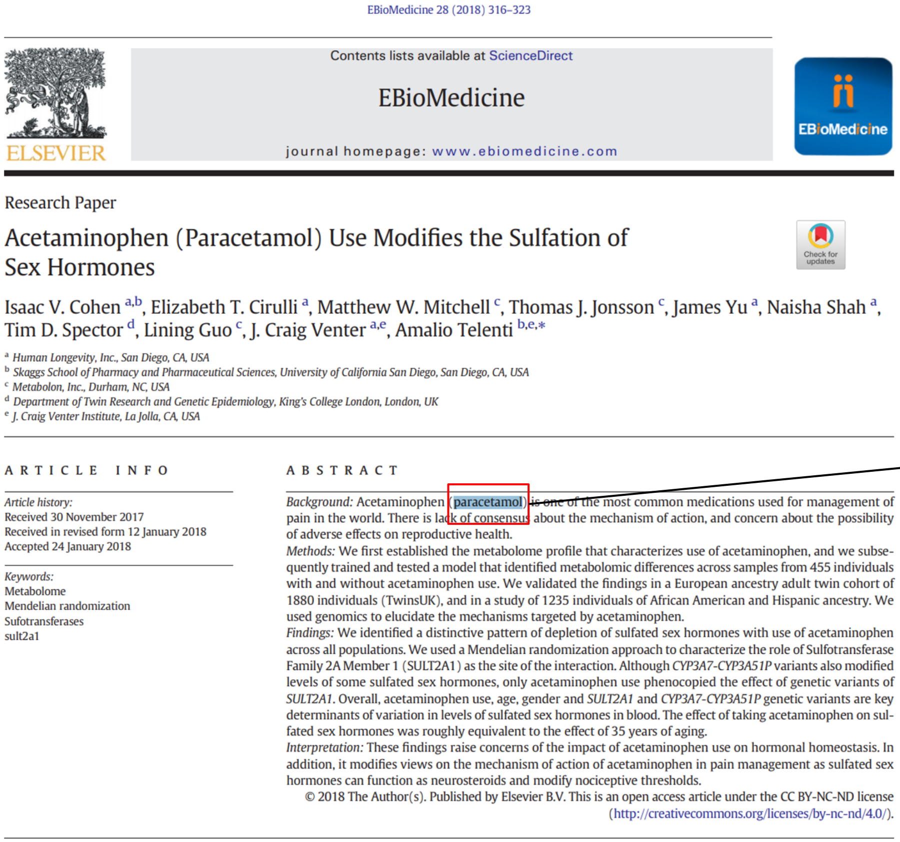
# LIBRETTI

NER + NEL



driven by excellence

## NER + NEL



EBioMedicine 28 (2018) 316–323

Contents lists available at ScienceDirect

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journal homepage: www.ebiomedicine.com

Research Paper

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[c] Metabolon, Inc., Durham, NC, USA
[d] Department of Twin Research and Genetic Epidemiology, King's College London, London, UK
[e] J. Craig Venter Institute, La Jolla, CA, USA

ARTICLE INFO

*Article history:*
Received 30 November 2017
Received in revised form 12 January 2018
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*Keywords:*
Metabolome
Mendelian randomization
Sufotransferases
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.

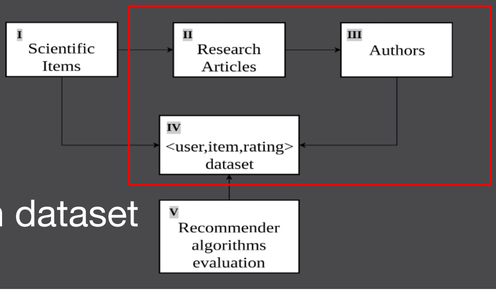
*Findings:* We identified a distinctive pattern of depletion of sulfated sex hormones with use of acetaminophen across all populations. We used a Mendelian randomization approach to characterize the role of Sulfotransferase Family 2A Member 1 (SULT2A1) as the site of the interaction. Although *CYP3A7-CYP3A51P* 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.

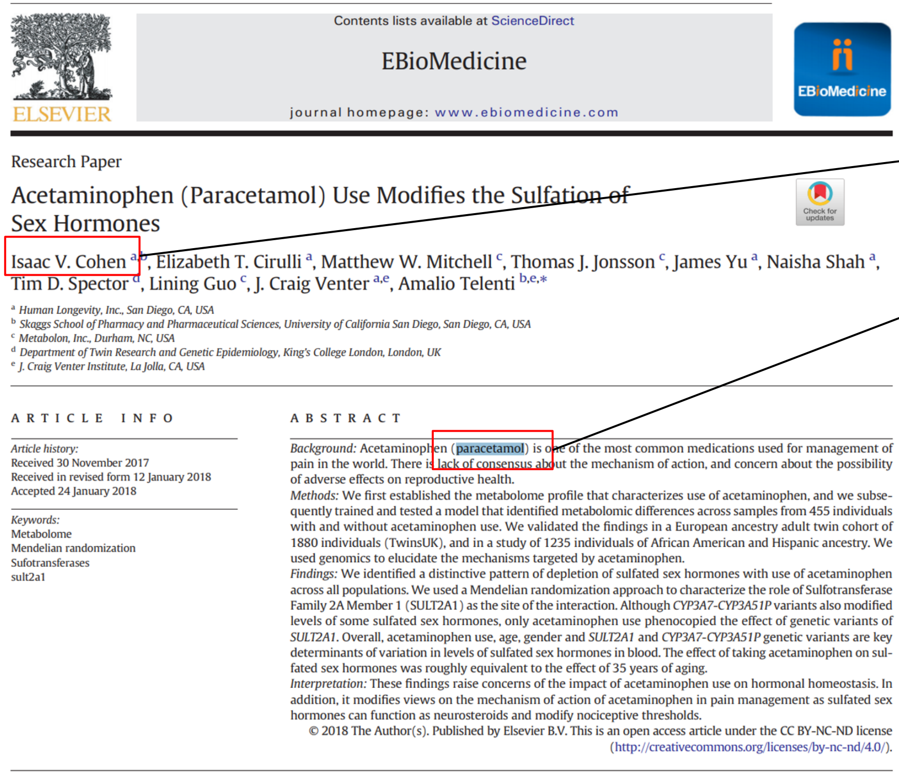
*Interpretation:* These findings raise concerns of the impact of acetaminophen use on hormonal homeostasis. In addition, it modifies views on the mechanism of action of acetaminophen in pain management as sulfated sex hormones can function as neurosteroids and modify nociceptive thresholds.

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

# LIBRETTI

From the articles to the recommendation dataset





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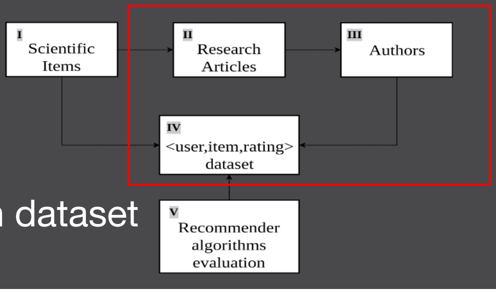
| User | Item | Rating |
|---|---|---|
| Isaac Cohen | Paracetamol | 1 |
| Elizabeth Cirulli | Paracetamol | 1 |
| Matthew Mitchell | Paracetamol | 1 |
| Thomas Jonsson | Paracetamol | 1 |
| James Yu | Paracetamol | 1 |
| Naisha Shah | Paracetamol | 1 |
| Tim Spector | Paracetamol | 1 |
| Lining Guo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

# LIBRETTI

From the articles to the recommendation dataset



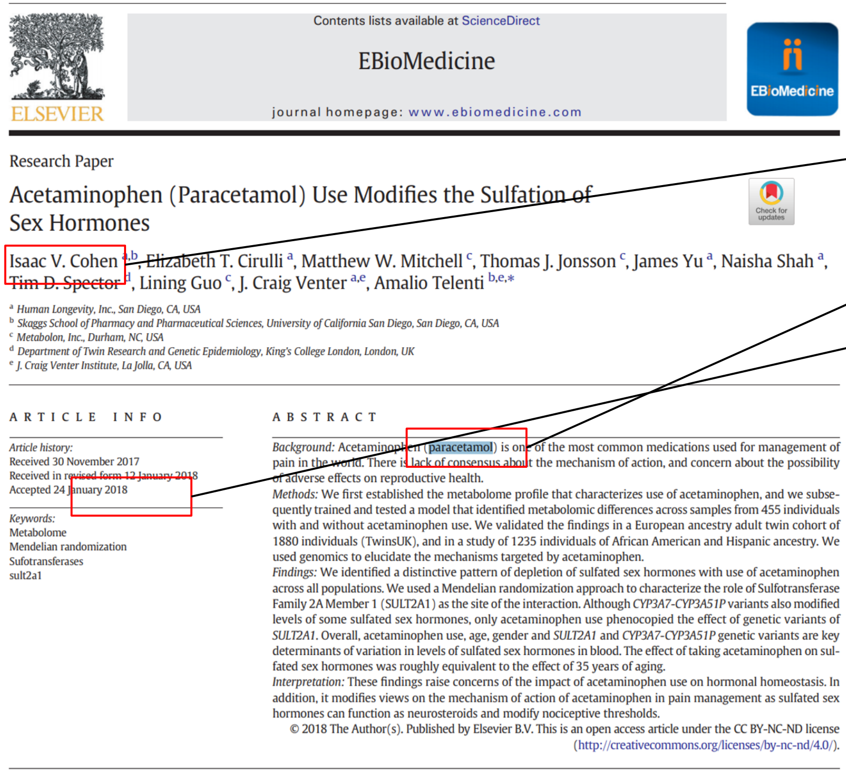
I Scientific Items

II Research Articles

III Authors

IV <user,item,rating> dataset

V Recommender algorithms evaluation



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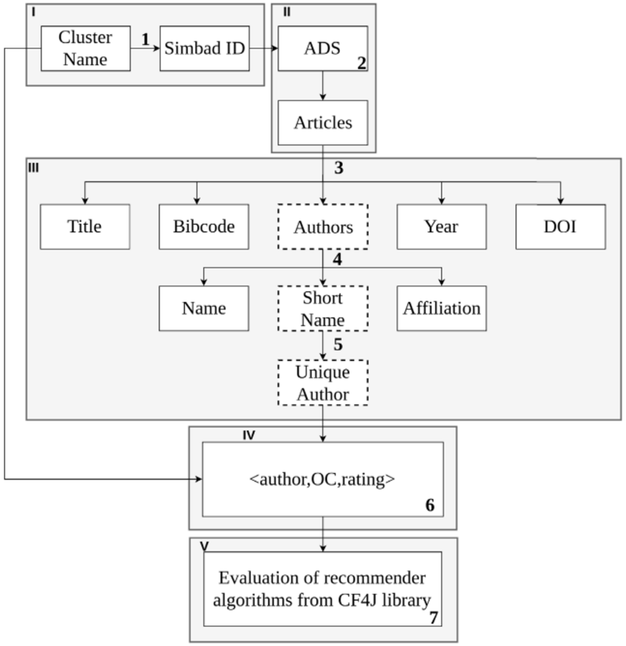
*Background:* Acetaminophen (paracetamol) is one of the most common medications used for management of pain in the world. There is lack of consensus about the mechanism of action, and concern about the possibility of adverse effects on reproductive health.
*Methods:* We first established the metabolome 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.

| 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 |

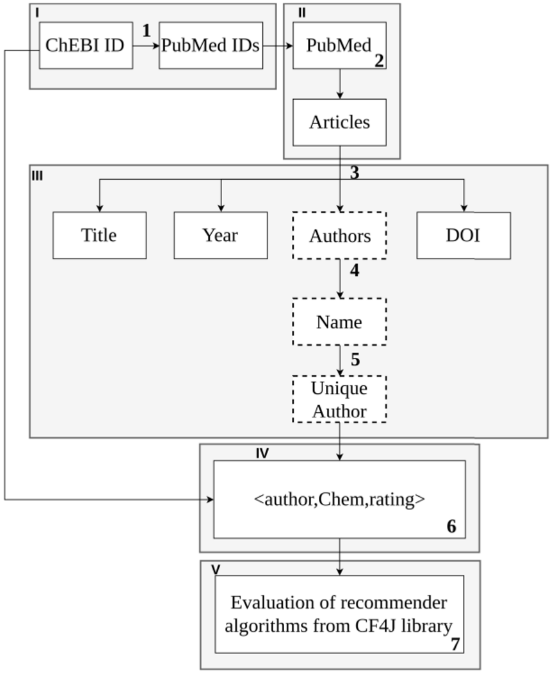
# LIBRETTI

Application fields

## Astronomy



## Chemistry



Barros, Márcia, André Moitinho, and Francisco M. Couto. "Using Research Literature to Generate Datasets of Implicit Feedback for Recommending Scientific Items." IEEE Access 7 (2019): 176668-176680. Q1 Scimago

# LIBRETTI

Application fields

## 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

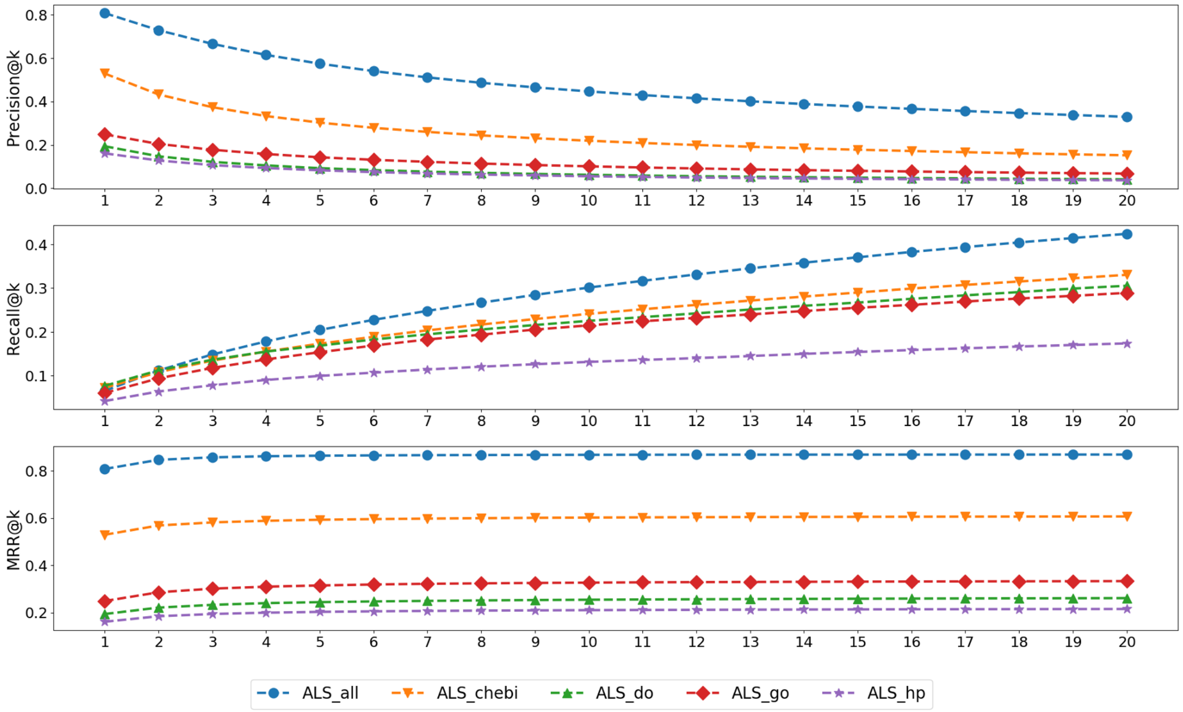
Barros, M. A., Lamurias, A., Sousa, D. F., Ruas, P., & Couto, F. M. (2020). COVID-19: A Semantic-Based Pipeline for Recommending Biomedical Entities. Proceedings of the 1st Workshop on NLP for COVID-19 (Part 2) at EMNLP 2020

# LIBRETTI

Application fields

## COVID-19

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.

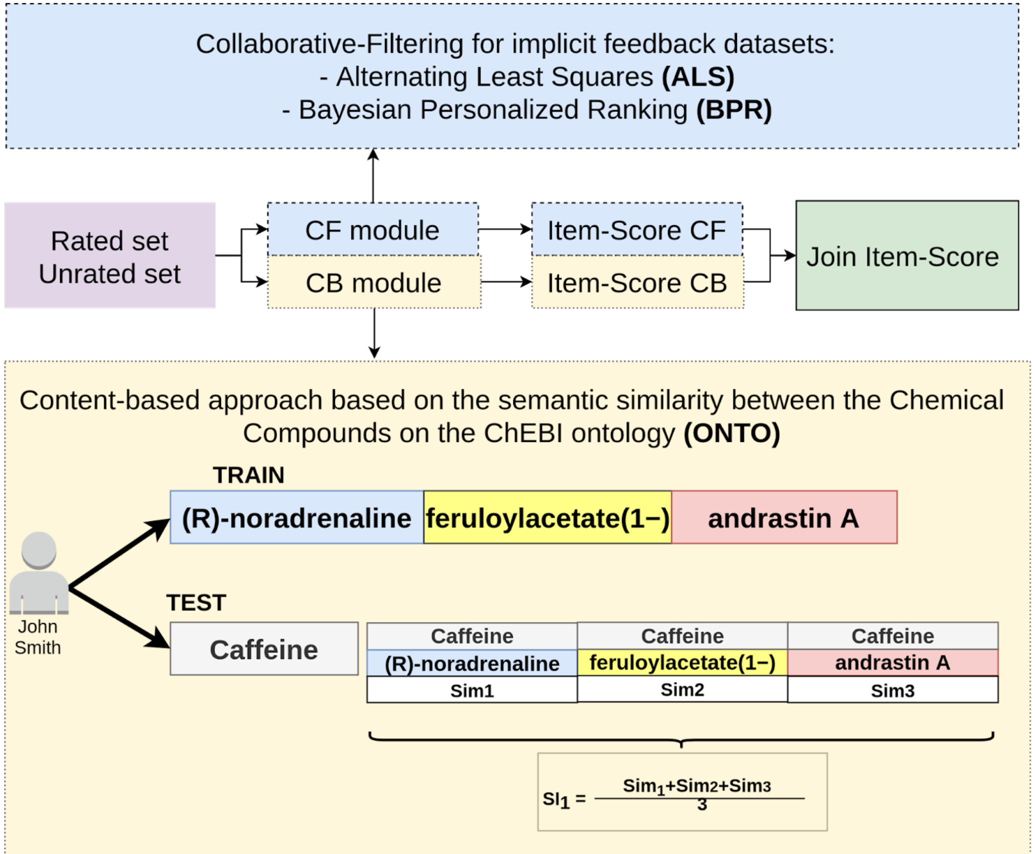


Barros, M. A., Lamurias, A., Sousa, D. F., Ruas, P., & Couto, F. M. (2020). COVID-19: A Semantic-Based Pipeline for Recommending Biomedical Entities. Proceedings of the 1st Workshop on NLP for COVID-19 (Part 2) at EMNLP 2020

# LIBRETTI

Developed methods

## ONTO



Collaborative-Filtering for implicit feedback datasets:
- Alternating Least Squares **(ALS)**
- Bayesian Personalized Ranking **(BPR)**

Rated set
Unrated set

CF module

CB module

Item-Score CF

Item-Score CB

Join Item-Score

Content-based approach based on the semantic similarity between the Chemical Compounds on the ChEBI ontology **(ONTO)**

**TRAIN**

| (R)-noradrenaline | feruloylacetate(1−) | andrastin A |
|---|---|---|

John Smith

**TEST**

Caffeine

| Caffeine | Caffeine | Caffeine |
|---|---|---|
| (R)-noradrenaline | feruloylacetate(1−) | andrastin A |
| Sim1 | Sim2 | Sim3 |

$$SI_1 = \frac{Sim_1+Sim2+Sim3}{3}$$

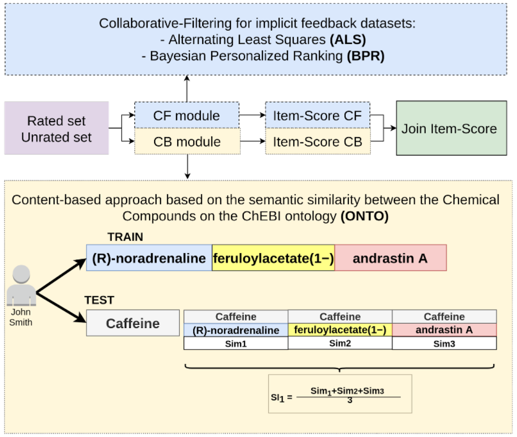
**Chemistry**

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.

# LIBRETTI

Developed methods

## ONTO



Collaborative-Filtering for implicit feedback datasets:
- Alternating Least Squares **(ALS)**
- Bayesian Personalized Ranking **(BPR)**

Rated set
Unrated set

CF module → Item-Score CF

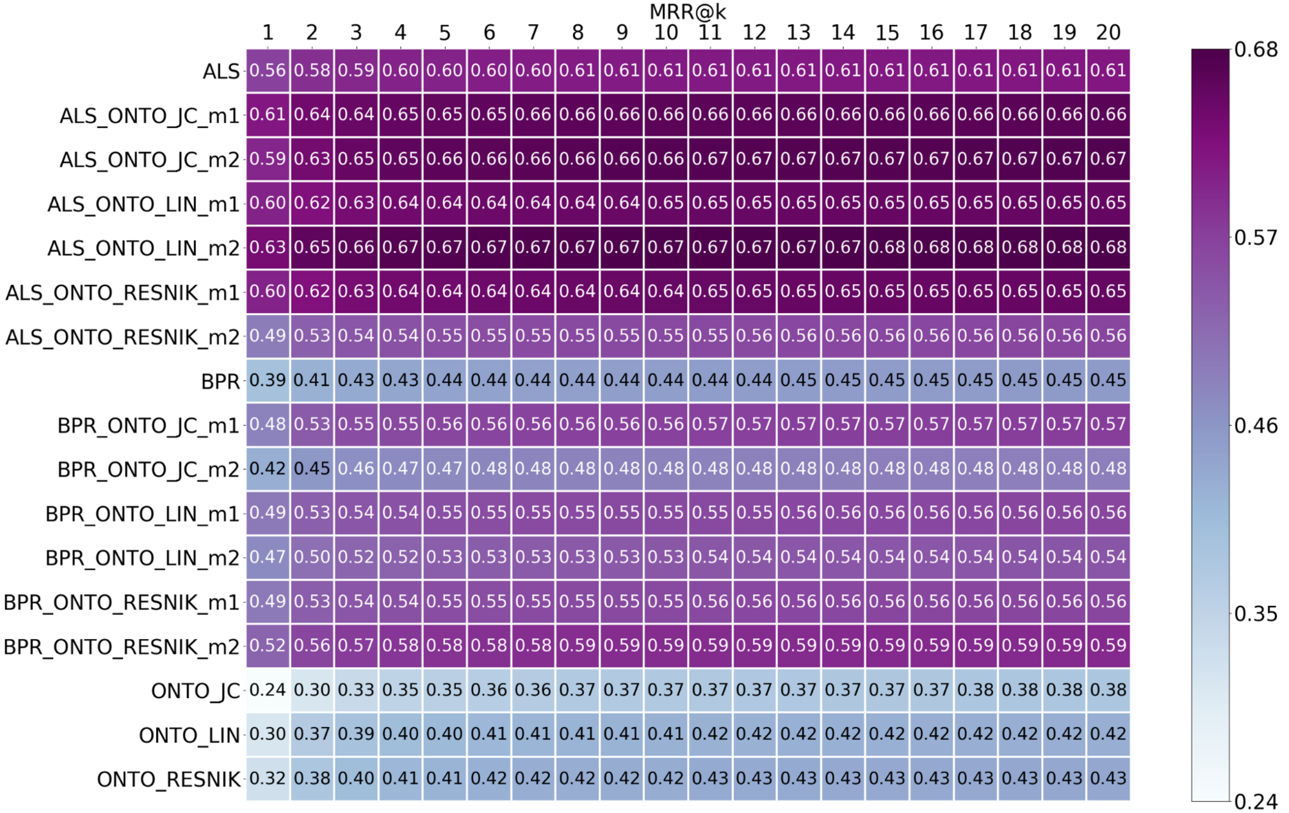
CB module → Item-Score CB

Join Item-Score

Content-based approach based on the semantic similarity between the Chemical Compounds on the ChEBI ontology **(ONTO)**

| Caffeine | Caffeine | Caffeine |
|---|---|---|
| (R)-noradrenaline | feruloylacetate(1−) | andrastin A |
| Sim1 | Sim2 | Sim3 |

$SI_1 = \frac{Sim_1+Sim2+Sim3}{3}$



MRR@k

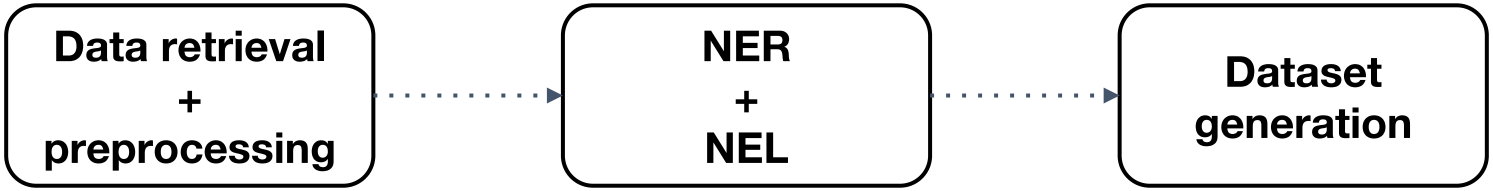
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ALS | 0.56 | 0.58 | 0.59 | 0.60 | 0.60 | 0.60 | 0.60 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 | 0.61 |
| ALS_ONTO_JC_m1 | 0.61 | 0.64 | 0.64 | 0.65 | 0.65 | 0.65 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 |
| ALS_ONTO_JC_m2 | 0.59 | 0.63 | 0.65 | 0.65 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.66 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 |
| ALS_ONTO_LIN_m1 | 0.60 | 0.62 | 0.63 | 0.64 | 0.64 | 0.64 | 0.64 | 0.64 | 0.64 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 |
| ALS_ONTO_LIN_m2 | 0.63 | 0.65 | 0.66 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.67 | 0.68 | 0.68 | 0.68 | 0.68 | 0.68 | 0.68 |
| ALS_ONTO_RESNIK_m1 | 0.60 | 0.62 | 0.63 | 0.64 | 0.64 | 0.64 | 0.64 | 0.64 | 0.64 | 0.64 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 | 0.65 |
| ALS_ONTO_RESNIK_m2 | 0.49 | 0.53 | 0.54 | 0.54 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 |
| BPR | 0.39 | 0.41 | 0.43 | 0.43 | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 | 0.44 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 | 0.45 |
| BPR_ONTO_JC_m1 | 0.48 | 0.53 | 0.55 | 0.55 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.57 | 0.57 | 0.57 | 0.57 | 0.57 | 0.57 | 0.57 | 0.57 | 0.57 | 0.57 |
| BPR_ONTO_JC_m2 | 0.42 | 0.45 | 0.46 | 0.47 | 0.47 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 | 0.48 |
| BPR_ONTO_LIN_m1 | 0.49 | 0.53 | 0.54 | 0.54 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 |
| BPR_ONTO_LIN_m2 | 0.47 | 0.50 | 0.52 | 0.52 | 0.53 | 0.53 | 0.53 | 0.53 | 0.53 | 0.53 | 0.54 | 0.54 | 0.54 | 0.54 | 0.54 | 0.54 | 0.54 | 0.54 | 0.54 | 0.54 |
| BPR_ONTO_RESNIK_m1 | 0.49 | 0.53 | 0.54 | 0.54 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.55 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 | 0.56 |
| BPR_ONTO_RESNIK_m2 | 0.52 | 0.56 | 0.57 | 0.58 | 0.58 | 0.58 | 0.58 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 | 0.59 |
| ONTO_JC | 0.24 | 0.30 | 0.33 | 0.35 | 0.35 | 0.36 | 0.36 | 0.37 | 0.37 | 0.37 | 0.37 | 0.37 | 0.37 | 0.37 | 0.37 | 0.37 | 0.38 | 0.38 | 0.38 | 0.38 |
| ONTO_LIN | 0.30 | 0.37 | 0.39 | 0.40 | 0.40 | 0.41 | 0.41 | 0.41 | 0.41 | 0.41 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 |
| ONTO_RESNIK | 0.32 | 0.38 | 0.40 | 0.41 | 0.41 | 0.42 | 0.42 | 0.42 | 0.42 | 0.42 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 | 0.43 |

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.

# PART 2

# How to build a scientific recommendation dataset?

Tutorial sections



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

# THANK YOU!!!