A large dataset of software mentions in the biomedical literature

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Abstract

We describe the CZ Software Mentions dataset, a new dataset of software mentions in biomedical papers. Plain-text software mentions are extracted with a trained SciBERT model from several sources: the NIH PubMed Central collection and from papers provided by various publishers to the Chan Zuckerberg Initiative. The dataset provides sources, context and metadata, and, for a number of mentions, the disambiguated software entities and links. We extract 1.12 million unique string software mentions from 2.4 million papers in the NIH PMC-OA Commercial subset, 481,000 unique mentions from the NIH PMC-OA Non-Commercial subset (both gathered in October 2021) and 934,000 unique mentions from 3 million papers in the Publishers’ collection. There is variation in how software is mentioned in papers and extracted by the NER algorithm. We propose a clustering-based disambiguation algorithm to map plain-text software mentions into distinct software entities and apply it on the NIH PubMed Central Commercial collection. Through this methodology, we disambiguate 1.12 million unique strings extracted by the NER model into 97,600 unique software entities, covering 78% of all software-paper links. We link 185,000 of the mentions to a repository, covering about 55% of all software-paper links. We describe in detail the process of building the datasets, disambiguating and linking the software mentions, as well as opportunities and challenges that come with a dataset of this size. We make all data and code publicly available as a new resource to help assess the impact of software (in particular scientific open source projects) on science.

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1. Introduction

The common adage says that the work of the scientist is only as good as their tools. While the last century software has become a key tool in a scientist’s toolbox and in recent years some of the most important breakthroughs in science—from the solution of 50-year-old protein folding problem [1] to the first-ever direct image of a black hole’s event horizon [2]—have been made possible through advanced computational methods applied to large swaths of data. Yet, identifying and crediting the computational tools that enabled these discoveries, and rewarding their creators, remains a challenge. While there are established norms in science for giving formal citation and credit to the authors of scholarly papers going back centuries, software—as many types of non-traditional research outputs [3, 4, 5]—is often neglected or treated as a second-class type of output and eminently hard to cite. Not being able to measure the impact of critical software tools that enable scientific progress makes it hard for their authors and maintainers to pursue scientific careers and to obtain funding for their work [6, 7, 8, 9, 10]. Furthermore, it makes it more difficult for other scientists to reproduce results in scientific papers, and creates barriers for funders who need to objectively evaluate the impact of their support [9, 11, 12, 13, 14].

While these problems have been well recognized [15, 9], and a number of recommendations for citing software have been published [16, 17], in scientific papers software is often only credited with informal mentions and phrases like for analysis ImageJ software was used. Until citation practices for software are improved, an analysis of the text of the papers remains necessary in order to get insight into software usage.

The extraction of software mentions from the text of scientific papers has attracted the attention of researchers for quite some time (see the review [18] and the recent publications [19, 20]). There are several datasets available, including SoftwareKG, a knowledge graph that contains information about software mentions from more than 51,000 scientific articles from the social sciences [21]; SoMeSci, a curated collection of 3756 software mentions in 1367 PubMed Central articles [22]; Softcite, a dataset of manual annotations of 4971 academic PDFs in biomedicine and economics [23]; [24], a dataset of 318,138 software mentions
based on CORD-19 dataset; and [25], another dataset of 77,449 software mentions based on CORD-19 dataset. These datasets are based on limited samples of scholarly articles. A paper based on a similar approach [26] was published while this preprint was in preparation. Similarly to our work, it is based on Pubmed Central Open Access dataset. The methodology for software extraction is similar and based on SciBERT [27]. The paper uses a hierarchical multi-task labeling model to extract additional tags besides software and the version, such as software type, mention type and additional information. The training corpora for our datasets are different: we trained our model on SoftCite [23], while Schindler et al. trained the model on the SoMeSci dataset [22]. Our disambiguation methodologies are overall similar and built on clustering algorithms, with differences in the type of features used. There is also a difference in the number of clusters obtained. Our linking methodology is quite different. The authors predict links based on training on the SoMeSci dataset, whereas we predict links by querying a number of repositories on names of clusters obtained through disambiguation. The authors extract 301,825,757 triples describing 11.8M software mentions and construct a knowledge graph based on the results. The sizes of the resulting mention datasets are similar: ours has 19.3M mentions (Table 1). The formats of the final datasets are also different: for example, we provide context for each mention in the dataset. We plan to conduct a more detailed comparison of our results and methods.

In this work we describe a series of larger datasets of software mentions based on (1) the full PubMed Central collection [28] downloaded in October 2021 containing more than 3.8 million papers (Table 1), and (2) a collection of papers provided by various publishers to the Chan Zuckerberg Initiative (Table 3). We use a SciBERT-based model trained on the SoftCite dataset [23] to extract software mentions from these corpora. There can be large variability in how a software entity is mentioned in text or extracted by the NER model, so we propose a clustering-based technique to disambiguate the plain-text mentions into distinct software entities (Section 2.4). We also describe a methodology to link the mentions to PyPI, CRAN, Bioconductor, SciCrunch or GitHub (Section 2.5).

We apply the disambiguation and linking methodologies to the PMC-OA comm subset, from which the NER model extracts 1.12 million unique string software mentions appeared in 2.4 million papers. We are able to disambiguate 320,000 of these mentions into 97,600 unique software entities, covering about 78% of all links in the dataset. For all the other strings extracted by the NER model, we cannot confidently map them to a software entity through our methodology. We also link about 185,000 mentions to a repository, covering about 55% of all software-paper links.

We curate a proportion of the final datasets by engaging a domain expert team. Through this process, we find that the precision of the NER model ‘in the wild’, on the top 10000 mentions (by frequency) in the PMC-OA comm subset, or Precision@10k is 69.66% (Precision score of the model on the SoftCite dataset is 90%). We describe in detail our methodology and make the final datasets available to the community. We hope this work serves as a resource for assessing the impact of scientific software.

2. Materials and Methods

2.1. Full text collection

We used two separate full text collections. The first dataset is based on the PubMed Central collection [28] (PMC OA) downloaded on October 2021. The PMC OA collection has two subsets: comm subset licensed for both commercial and non-commercial use, and non-comm subset licensed for non-commercial use only, including data mining. We kept these data separate to ensure that our data set can be utilized for both commercial and non-commercial uses (see the discussion of non commercial licensing in [29]). The statistics of the data set is shown in Table 2. Second, there were full-text manuscripts of scholarly articles (both Open Access and paywalled manuscripts) provided to the Chan Zuckerberg Initiative by publishers under different agreements (Publishers’ collection). This corpus also includes preprints from bioRxiv. The provenance and time span of this collection varies (see Table 3). As seen from Tables 3 and 1, the datasets have significant overlap.

The Publishers’ collection was stored in LXML format PMC OA papers were downloaded in NXML format. For parsing LXML we used lxml [30]; for parsing NXML we used a modified pubmed_parser software [31]. Our modifications concerned table caption extraction (not implemented in the original) and speeding up parsing. They, along with the other modules, are available at the GitHub site accompanying this publication. The extracted text was fed into the SciBERT-based NER model (Section 2.2) and further processed (Section 2.4).

| Parameter                  | Commercial set | Non-commercial set |
|----------------------------|----------------|---------------------|
| Number of papers           | 2,433,010      | 1,442,868           |
| Number of papers with at least one mention | 1,732,603     | 758,246             |
| Number of mentions         | 14,770,209     | 4,546,607           |
| Number of unique mentions  | 1,120,125      | 481,972             |
Table 2: Publishers collection statistics

| Parameter                  | Publishers Collection |
|----------------------------|-----------------------|
| Number of papers           | 16,809,266            |
| Number of papers with at least one mention | 2,893,518 |
| Number of mentions         | 48,160,836            |
| Number of unique mentions  | 934,704               |

2.2. Software Mentions Extraction

We use a NER model to extract plain-text software mentions from our corpus. The SciBERT [27] model has been fine-tuned on the SoftCite dataset [23] to recognize mentions of software and respective version. This model achieves a 10-fold cross-validation F1 score of 0.92. More details can be found at the address https://github.com/chanzuckerberg/software-mention-extraction. This model was previously used on the CORD-19 dataset [25].

For a part of the collection: OA PMC corpus released under free license for both commercial and non-commercial use (comm dataset) we performed linking and disambiguation described below.

2.3. Software Mentions Linking and Disambiguation

There can be large variability in how a piece of software is being mentioned in text (Figure 1). For example, a software can be mentioned through its full name (e.g. Statistical Package for Social Sciences) or its acronym (e.g. SPSS). There can also be multiple name variations commonly accepted as referring to the same software entity (e.g. sklearn and scikit-learn). And there can be variability in how a software mention is being mentioned by researchers (e.g. Image J and ImageJ or GraphPad Prism and GraphPad and Prism). Moreover, there can be typos, either introduced by the authors (e.g. scikits-learn) or by parsing the XML of the papers, and there can be variability in how the NER algorithm extracts different software mentions (e.g. partial matches). If we want to assess the impact of a software entity, we need to be able to map all of the different string variations that correspond to a particular software entity together.

Our goal is to build a software entity data model and describe a software entity through its name (e.g. scikit-learn, Figure 2), the string variations under which this entity appears mentioned in the literature, as extracted by the NER model (e.g. sklearn, Sklearn API, scikit-learn API, scikits-learn, Python toolbox scikit-learn, Scikit-Learn Library, etc) and, ideally, a link to a repository or database, such as https://pypi.org/project/scikit-learn.

To achieve this, after extracting the software mentions from the PMC-OA corpus using the NER model, we use two additional methodologies: disambiguation and linking for the part free for commercial use (Table 1). We define disambiguation as the process of mapping various string variations of the same software entity together. Linking refers to mapping a software entity to a URL in a repository or database. Our algorithm is shown as Algorithm 1. We describe each of these steps in more detail in the following sections.

2.4. Software Mentions Disambiguation

In the PMC-OA comm corpus, MATLAB, the R package limma and GraphPad are each extracted by the NER model under more than 200 string variations. BLAST, an algorithm for comparing primary biological sequence information, has more than 500 variations extracted by the NER model (see Figures 3 and 4 with additional examples in Appendix D). Through disambiguation, our goal is to group different string variations of the same software entity together. For instance, all the string variations for...
| Publisher                                                      | Number of papers with at least one mention |
|---------------------------------------------------------------|--------------------------------------------|
| American Association of Neurological Surgeons                | 7,512                                      |
| American College of Physicians                               | 1,001                                      |
| American Institute of Aeronautics and Astronautics           | 8,670                                      |
| American Institute of Physics                                | 48,565                                     |
| American Physical Society                                    | 9,649                                      |
| American Psychiatric Association Publishing                  | 5,171                                      |
| American Society for Clinical Investigation                  | 8,787                                      |
| American Society for Microbiology                            | 4,943                                      |
| American Society of Agricultural and Biological Engineers    | 1,132                                      |
| American Society of Civil Engineers                          | 30,641                                     |
| American Thoracic Society                                    | 2,247                                      |
| Annual Reviews                                                | 8,307                                      |
| BioOne                                                       | 61,832                                     |
| bioRxiv                                                      | 33,136                                     |
| Cambridge University Press                                   | 205                                        |
| CSIRO Publishing                                             | 5,999                                      |
| De Gruyter Open                                              | 4,603                                      |
| Edinburgh University Press                                   | 6,784                                      |
| eLife Sciences Publications, Ltd                             | 1,652                                      |
| Emerald Publishing Limited                                   | 55,367                                     |
| Future Medicine Ltd                                          | 18,934                                     |
| Hindawi                                                      | 23,052                                     |
| Hogrefe Publishing                                           | 8,067                                      |
| Impact Journals                                              | 4,191                                      |
| INFORMS                                                      | 669                                        |
| Institute of Electrical & Electronics Engineers              | 43,580                                     |
| IntechOpen                                                   | 1                                          |
| International Union of Crystallography                       | 21                                         |
| IOS Press                                                    | 3,989                                      |
| MA Healthcare                                                | 8,284                                      |
| Mary Ann Liebert, Inc., publishers                           | 65,597                                     |
| MDPI                                                         | 14,334                                     |
| MIT Press                                                    | 2,544                                      |
| Public Library of Science                                   | 186,313                                    |
| PubMed Central Open Access                                  | 1,758,247                                  |
| Royal College of Surgeons of England                         | 1,458                                      |
| Royal Society of Chemistry                                   | 73,586                                     |
| SAGE Publications                                            | 358,849                                    |
| SLACK Incorporated                                           | 2,801                                      |
| Society of Photo-Optical Instrumentation Engineers           | 31                                         |
| Springer Nature                                              | 329,910                                    |
| Taylor & Francis                                             | 607,702                                    |
| The Royal Society                                            | 342                                        |
| University of California Press                               | 457                                        |
| Wolters Kluwer                                               | 32,940                                     |
| Total                                                        | 3,852,092                                  |
Input Papers $P = P_1, P_2, ... P_n$
Output software,entities $\left\{ \right\}$

for $P_i \in P$ do
  $V_i \leftarrow \text{NER}(P_i)$ // strings extracted by the NER algorithm from $P_i$
end for

$S \leftarrow V_1 \cup V_2 \cup \ldots \cup V_n$ // set of all strings extracted
$M \leftarrow \text{get_similarity_matrix}(S)$
$C_1, C_2, ... C_n \leftarrow \text{get_connected_components}(M)$

for $C_i \in C_1, C_2, ... C_n$ do
  $M_i \leftarrow \text{get_similarity_matrix}(C_i)$
  $D_i \leftarrow 1 - M_i$ // distance matrix
  for Cluster $j \in \text{DBSCAN}(D_i)$ do
    $s_{jD_i} \leftarrow \text{highest_frequency_string}(\text{Cluster}_j)$
    software,entities[$s_{jD_i}$][‘variations’] $\leftarrow \text{Cluster}_j$
    software,entities[$s_{jD_i}$][‘link’] $\leftarrow \text{get_link}(s_{jD_i})$
  end for
end for

Algorithm 1: Disambiguation and linking

limma should be grouped under the limma software entity, all the string variations for MATLAB should be grouped under the MATLAB software entity, and so on.

Starting with a set of papers (in our case the PMC-OA corpus), we run the NER algorithm and obtain the set $S$ of all software strings extracted from the corpus. We build a similarity matrix $M$ containing similarity scores between pairs of strings in $S$. Then we break $M$ down into distinct connected components, and run DBSCAN [32] on each. From each connected component, we obtain clusters of strings corresponding to well-defined software entities. The final list of clusters is the union of all the clusters from each of the connected components in $M$. To obtain $M$, we use a combination of Keywords-based synonym generation, SciCrunch synonyms retrieval and Jaro-Winkler string similarity scores. We go over our methodology in more detail below.

2.4.1. Keywords-based Synonym Generation

We query PyPi [33], CRAN [34] and Bioconductor [35] indices, which contain lists of software packages available on each of these platforms. For each software entry in each index, we look for entries in the list of all plain-text software mentions that contain the match and keywords relevant to that index. For example, once we find limma as an entry in the Bioconductor package, we look for other plain-text software mentions in our original list that contain the word limma and keywords relevant to the Bioconductor index, such as limma R package, R package limma, etc. We consider pairs retrieved this way (e.g. limma and limma R package and limma and R package limma) to be high-confidence synonyms.

2.4.2. SciCrunch Synonyms Retrieval

We query the SciCrunch API [36] for each of the mentions in our corpus. When queried for a particular en-
Table 4: Keywords used for synonym generation

| Index       | Keywords Used                                                                 |
|-------------|-------------------------------------------------------------------------------|
| PyPI        | ['python', 'Python', 'API']                                                   |
| CRAN        | ['R', 'r', 'package', 'Package', 'R-package', 'R-Package', 'r-package']        |
| Bioconductor| ['R', 'r', 'package', 'Package', 'R-package', 'R-Package', 'r-package',       |
|             | 'bioconductor', 'Bioconductor']                                               |

Table 5: Examples of software synonym pairs retrieved through the SciCrunch API

| Software Mention     | Synonym                                              |
|----------------------|------------------------------------------------------|
| SPSS                 | Statistical Package for the Social Sciences          |
| SPSS                 | IBM SPSS                                             |
| SPSS                 | IBM SPSS Statistics: International Business Machines |
| BLASTN               | Standard Nucleotide BLAST                           |
| BLASTN               | Nucleotide BLAST                                    |
| BLASTN               | NCBI BLASTN                                         |
| BLASTN               | BLASTn                                               |

Table 6: Examples of software synonym pairs retrieved through keywords synonym generation. The synonyms are strings extracted by the NER algorithm

| Software Mention     | Synonym                                              |
|----------------------|------------------------------------------------------|
| scikit-learn         | scikit-learn python package                          |
| scikit-learn         | scikit-learn python library                          |
| scikit-learn         | scikit-learn python                                  |
| scikit-learn         | scikit-learn library for Python                      |
| scikit-learn         | scikit-learn Python package2223                      |
| scikit-learn         | scikit-learn Python package for                       |

Figure 4: Examples of string variability for the software ‘BLAST’ ([https://scicrunch.org/browse/resources/SCR_008419](https://scicrunch.org/browse/resources/SCR_008419)), as extracted by the NER model from the PMC-OA corpus.
string similarity [37] values in our matrix. We only use pairs of synonyms with a confidence $\geq 0.97$. We make this choice so that the largest connected component can fit into working memory and also to increase the confidence in the pairs of synonyms we consider. A drawback of this is that we will lose a number of pairs of synonyms. Future work could include finding ways to overcome this limitation. Our similarity matrix is described by:

$$M_{ij} = \begin{cases} 1, & (i, j) \in S_2 \\
0.99, & (i, j) \in S_1 - S_2 \\
n_{ij}, & \text{otherwise, and } n_{ij} \geq 0.97 \end{cases}$$

where $S_1$ is the set of pairs based on keywords-based generation, $S_2$ is the set of pairs obtained from SciCrunch, and $n_{ij}$ is Jaro-Winkler distance. We perform additional post-processing of $M$ in order to increase data quality for clustering. Steps we include are: assigning confidences of 1 for pairs of synonyms that are equal when stripped of digits, punctuation or copyright characters, or that have more than one word token and are equal, lowercase-insensitive. We also remove pairs that include broad terms that tend to have a lot of synonyms, such as ‘R package’, ‘r package’, or ‘interface’. Full details can be found in our code.

Once we have built our similarity matrix $M$ and post-processed it, we extract the connected components $C_1$, $C_2$, $\ldots$, $C_n$ of $M$ and then run the DBSCAN [32] algorithm on each similarity matrix $M^{(n)}$ corresponding to the component number $n$. Computing the connected components helps us to reduce the size of the matrix we have to run the clustering algorithm on. For each $M^{(n)}$ we compute a distance matrix $D^{(n)}$ such that

$$D^{(n)}_{ij} = 1 - M^{(n)}_{ij}.$$  

Using DBSCAN we obtain a set of clusters corresponding to each connected component in our graph. For each cluster, we select the software mention with the highest frequency in our corpus as the cluster name. Empirically, we noticed that this string variation is the most likely to be the real name of the software entity. This also corresponds to the intuitive idea of the “true software mention”.

Our algorithm is presented as Algorithm 2.

We use the textdistance python package [38] to compute the Jaro-Winkler similarity scores. We use a CSR sparse matrix format for the similarity matrix and use the connected_components module from scipy.sparse.csgraph [39] to obtain the connected components. We use the DBSCAN implementation from sklearn.cluster [40].

2.5. Software Mentions Linking

Once we cluster different software string variations together, we also want to link them to the corresponding URLs. For each software mention in our corpus, we do an exact match search in the PyPI [33], CRAN [34] and Bioconductor [35] indices, as well as GitHub [41] and SciCrunch [42] APIs. For PyPI, CRAN, Bioconductor and SciCrunch, we also query individual URL pages for matches we find. Combined, we obtain links, as well as additional metadata, for a number of software mentions. Because the format and type of metadata available varies across repositories, we normalize the formats to a common schema between repositories. The final metadata fields we retrieve across repositories and normalizing to contain: source, package_url, description, homepage_url, other_url, license, github_repo, github_repo_license, exact_match, RRID, reference. Note that not all software mentions will have all of the metadata fields present, either because there was no corresponding field in the database for that field, or the entry was empty in the database. We make the schema normalization mappings between the initial fields present in a database and the final metadata fields available in Table 7 and Appendix A.

We map each cluster to the link to which the cluster name is pointing to. For instance, we map all the entries in the scikit-learn cluster to the scikit-learn link. For situations where the cluster name does not have an associated link, or a software mention is not mapped to a cluster, we look for an exact match link for that particular software mention itself.

2.6. Dataset Curation

2.6.1. Motivation

The NER model has an F1 score of 0.922, with a precision of 0.9063 and a recall value of 0.9385. These metrics are calculated on the SoftCite dataset [23], which has been used for training the NER model. Since the PMC-OA corpus distribution is different from the one of the SoftCite Dataset, we engaged our in-house team of bio-curators to first evaluate a sample of the top 1000 plain text software mentions (by means of frequency) extracted from the PMC-OA comm subset. Based on this evaluation, we concluded that the Precision@1000 of the NER model “in the wild”, on the PMC-OA corpus is 79.5%. After this assessment, and in order to eliminate as much noise from the dataset as possible, we engaged our bio-curator team to

Input distance matrices $D^{(n)}_{ij}$

Output all_clusters $\leftarrow \{\}$

for all connected components $C_n$ of $M$ with distance matrices $D^{(n)}_{ij}$ do

Cluster$^{(n)}_1$, Cluster$^{(n)}_2$, $\ldots$ $\leftarrow$ DBSCAN($D^{(n)}$)

for all clusters Cluster$^{(n)}_i$ from component $C_n$ do

Select vertex $s^{(n)}_i$ $\in$ Vertices(Cluster$^{(n)}_i$) with the highest frequency on PMC-OA comm

Name(Cluster$^{(n)}_i$) $\leftarrow$ $s^{(n)}_i$

all_clusters $\leftarrow$ all_clusters $\cup$ Cluster$^{(n)}_i$

end for

end for

Algorithm 2: Clustering and naming
We want to note that the relatively low IAA value demonstrates our IAA values of concern are around 0.639/0.686. Since we are considering five subcategories (software, algorithm, database, web platform, and the NER model was trained. We start with five different categories: software, algorithm, database, web platform, and other and ask our curators to annotate the top 1000 most frequent mentions from our corpus with these categories. To facilitate the curation process, we provide for each software mention five different sentences extracted from the articles; where the sentences do not provide sufficient information about the software, the curators are asked to find background information through Google searches. The curation of the top 1000 mentions allowed us to (a) understand the variety of mentions that are present in the dataset (see Table 10) and (b) identify additional examples for each category (in particular, borderline cases) and refine the curation guidelines further.

We consider mentions in the software and algorithm categories to be true software, whereas mentions in the database, hardware, web platform and other categories are considered as non-software. Based on this human evaluation, 79.5% of 1000 mentions are evaluated as software, and 16.5% as non-software. For the remaining 4% of mentions, a distinction between software and non-software could not be made; this is either because a software name or acronym could be pointing to two different entities (labeled as unclear), or because the mentions extracted by the NER model were random symbols. For the evaluation of the 9000 mentions, we only ask our curators to distinguish between the main software/non-software categories. We provide more detailed curation guidelines in Appendix B. In the final curated dataset of 10000 software mentions, 69.66% of mentions are evaluated as software, 21.55% as non-software, and for 8.79% an evaluation could not be made.

2.6.3. Inter-Annotation Agreement

We compute the Inter-Annotation Agreement (IAA) value by looking at curator evaluations on a random sample of 100 mentions from the larger sample of 1000 (Table 10). With four curators per mention, we obtain a Fleiss Kappa IAA value [43] of 0.639 when only the two main categories (software/non-software) are considered, and 0.504 when the more specific five subcategories (software, algorithm, database, web platform, hardware, other) are labeled. We also compute the Krippendorff Alpha IAA [43] values, which are similar: 0.686 for the two main categories and 0.523 for five subcategories (Table 11). Since we are interested in the binary (software/non-software) differentiation, our IAA values of concern are around 0.639/0.686. We want to note that the relatively low IAA value demon-
strates that this is a challenging task even for our expert curator team. The fact that the IAA value is relatively low should be interpreted as a signal for how hard it is to distinguish in some cases whether a mention is a true software or not. Specifically, it is difficult to differentiate between ‘software’ and ‘algorithm’ as these terms are often used interchangeable by authors describing their tools: the tool may be called “software” on the tool’s website but described as an “algorithm” in an article. Similarly, some online tools consist of a database and software of the same name, so there may be disagreement how curators annotate the software mention. It is also important to note that the curation relied on both the context given by 5 example sentences and background searches. The use of different sources of information can result in different annotations; this is particularly true for software mentions that consist of acronyms, have ambiguous names or share part of their name with other software and/or non-software resources.

3. Evaluation & Results

3.1. Final Dataset

The statistics of software mentions extracted from the OA-PMC comm dataset is shown in Table 1. The results of disambiguation and linking are shown in Table 12. As seen from this table, for about 390,000 mentions we could not generate synonyms or we discarded them during post-processing. By analyzing some of these mentions, we hypothesize that they are likely to be noise or false positives. For about 720,000 mentions we were able to generate synonyms. Again, about 400,000 of the latter were too ambiguous to disambiguate. This is likely because the software mentions did not have significant synonyms (with a confidence of ≥ 0.97 during the disambiguation phase). The remaining 320,000 mentions were mapped into 97,600 unique software entities through the disambiguation algorithm. This covers 78% of all links in the dataset. Lastly, for about 185,000 mentions we were able to obtain links to GitHub, PyPI, CRAN, Bioconductor, or SciCrunch. This covers about 55% of all software-paper links.

3.2. Disambiguation

Perhaps the biggest challenge in disambiguation is that we don’t have curated labels to learn from. Our methodology, based on DBSCAN [32], is unsupervised. We engaged our biocurators for evaluation of the results.

We created a set of 5884 pairs of generated synonyms coming from 104 unique software mentions for manual curation. This dataset was generated from an initial iteration of the disambiguation algorithm. We asked our curation team to label each synonym pair with one of the following categories:

- **Exact**: synonym is an exact match of the assigned Software mention
- **Narrow**: synonym is a child term
- **Not Synonym**: synonym is an unrelated software or other term

The Exact category includes all mentions that can unambiguously be assigned to the software mention, including partial terms, typos, variations on spelling (upper/lower case, space, hyphen etc), and acronyms. Reference numbers in the article are often erroneously added to the software synonym; these are also labeled as Exact. Versions of software are annotated as Narrow. Partial versions are also included here, for example “Autodock Vina1” for “Autodock Vina1.1.2”. It is worth noting that synonyms representing software versions can be challenging to distinguish from synonyms which include the reference number (e.g. “Autodock Vina19” where 19 is the reference number in the article mentioning the software). Synonyms of software tools that have common names pose another challenge for this task: for example, it is time-consuming to work out whether “ClusterM” is a true synonym for a version of the software tool “Cluster” or represents a completely distinct software called ClusterM. We considered pairs that fall into either of Exact or Narrow categories to be true synonyms. Composition of this curated labels is under (Table 13).

We used this dataset and the labels assigned by our curators to validate our clustering technique, by computing the Precision, Recall and the F1 score for generated pairs of synonyms. We chose the hyperparameters that gave the highest metrics on this curated dataset. Our best model had an F1 score of 0.704, with a Precision of 0.954 and Recall of 0.558.

We offer some examples of disambiguated terms obtained through DBSCAN clustering for the scikit-learn, ImageJ and SPSS software entities in Figure 5, Figure 6 and Figure 7.
### Table 12: OA PMC comm disambiguation and linking

| Category               | Mentions | Paper-software links | Notes                                      |
|------------------------|----------|----------------------|--------------------------------------------|
|                        | Approx. # | %                    | Approx. # | %                        |
| undisambiguated        | 393,057  | 35 %                 | 731,529  | 8.95 %                   |
| undisambiguated        | 404,493  | 36.11 %              | 1,050,017 | 12.85 %                 |
| disambiguated          | 323,561  | 28.88 %              | 6,384,430 | 78.18 %                 |
| disambiguated and linked | 185,427  | 16.55 %              | 4,555,476 | 55.78 %                 |
| total unique mentions  | 1,120,111 | 100 %               | 8,165,976 | 100 %                   |

**Table 13: Disambiguation Evaluation.** Description of the dataset used for evaluating disambiguation. Labels were assigned by our curation team on 5886 pairs of generated synonyms coming from 103 unique software mentions

| Synonym Pair Label | Count | %       |
|--------------------|-------|---------|
| Correct - Exact    | 3147  | 53.465  |
| Correct - Narrow   | 1094  | 18.586  |
| Incorrect          | 668   | 13.484  |
| Unclear            | 45    | 0.908   |
| Not software       | 930   | 15.805  |

### 3.3. Linking

As with disambiguation, we don’t have any labeled data to evaluate our linking, so we engage our team of biocurators for feedback. We provide our biocurators with 50 software mentions, together with the generated links. Based on biocurator feedback, 54% of the generated links are correct, 6% are incorrect, and for 40% it is unclear whether the link is correct. Most notably, 39/40 mentions for which the link is unclear are retrieved from GitHub and only one is linked through PyPI, Bioconductor, CRAN and SciCrunch. This happens because GitHub is a resource that is not curated, so having an exact match on a software name in GitHub does not guarantee that it will be linking to the actual software. Anyone can upload software in GitHub and name it as they wish. A number of repositories we evaluated were empty, or contained too little information to be able to decide for sure if the linking was correct. When we consider the evaluation only of links retrieved through PyPI, Bioconductor, CRAN and SciCrunch, the accuracy improves considerably: 93.33% of links are correct and 0.6% are incorrect, 0% unclear. This suggests that linking software through these four repositories through an exact match is likely to give correct links. We note, however, that the sample size for this evaluation is quite small, and it is possible that results might change with a larger sample.

### Table 14: Linking Coverage

| Repository           | Number of linked mentions | %   |
|----------------------|---------------------------|-----|
| GitHub API           | 155,506                   | 64.39 |
| SciCrunch API        | 43,817                    | 18.14 |
| CRAN                 | 20,202                    | 8.36 |
| PyPI                 | 14,154                    | 5.86 |
| Bioconductor         | 7,801                     | 3.23 |

### Table 15: Linking Evaluation on a sample dataset of 50 generated links to PyPI, CRAN, Bioconductor, GitHub and SciCrunch

| Link label | All links | Excluding GitHub | %   |
|------------|-----------|------------------|-----|
| correct    | 27        | 14               | 93.33 |
| unclear    | 20        | 1                | 6.66 |
| incorrect  | 3         | 0                | 0   |

5. Discussion

The dataset we make available is, to our knowledge, the largest dataset of software mentions in the scientific literature currently available. In this section, we go over some of the lessons learned in building a dataset this large, as well as limitations of current work. We offer a view on opportunities for further work in the Next Steps section.

#### 5.1. Extraction

An important feature of our extraction is the maximal preservation of the context of the software mention. We keep the sentence from which the mention was extracted as well as the reference to the unit (section, caption, abstract) from which it was extracted. This helped in the curation. This may facilitate more deep reprocessing of the dataset in the future, including better disambiguation and linking.

4. Code & Data Availability

We make the dataset, as well as all intermediate files available at [https://doi.org/10.5061/dryad.6wzpzn2c](https://doi.org/10.5061/dryad.6wzpzn2c) under a CC0 license [44]. All the code used for extraction, disambiguation and linking, as well as instructions on how to reproduce the results and some starter code is available at a GitHub repository [https://github.com/chanzuckerberg/software-mentions](https://github.com/chanzuckerberg/software-mentions) under the MIT license with the permanent snapshot at [45].
Cluster: ‘scikit-learn’

Scikit-Learn
scikit-learn Python
scikit-learn
Scikit learn
sklearn
scikit-learn Python library
Scikit-learn
Sklearn
Python scikit-learn
scikit learn
scikit-learn
Scikit-learn
Scikit-Learn Python
scikit-learn81
SciKit-Learn
sklearn Python
SkLearn
scikit -learn
Python Scikit-Learn
Scikit-Learn®
Python sklearn library
scikit.learn
Scikits-learn
Sci-kit-learn
scikit-learn Python3 package
Sci-Kit learn
sklearn0
Python Scikit Learn
Scikit-Learn Python Library
Python scikit_learn
2scikit-learn
SCikit-learn
SCIKIT-learn
Scikit–Learn
Python Scikit learn
Python package Scikit-learn
scikit-Learn
Scikit-Learn Python package
scikit-learn Python Library
sklearn python package
sci-kit learn Python package
Python scikit learn package
skLearn
Scikit-learn python
scikitslearn
scikit-learn Python package for
Python scikit learn
Scikit–Learn Python
scikit - learn Python library

Figure 5: Sample of Disambiguation results for the software entity scikit-learn. There are a total of 124 unique string variations extracted by the NER model that are mapped to the scikit-learn software entity through disambiguation.

Cluster: ‘ImageJ’

ImageJ
Image J
image J
Image-J
Image J1
Image J2
Image J©
Image/J®
image-j
IMAGE-J
ImageJ (Image Processing and Analysis in Java
Image-j
Image J)
IMAGE j/
ImAgeJ
imageJ1
Image -J
ImageJ®1
Image,J, Image Processing and Analysis in Java
ImageJ (Image Processing and Analysis in Java)
ImageJ Image Processing and Analysis in Java
ImageJ-145
image J1
IMageJ1
imageJ64
ImageJ -
ImageJ)
ImageJ®
Image/J
Image J-Image Processing and Analysis in Java
Image J- Image Processing and Analysis in Java’

Figure 6: Sample of Disambiguation results for the software entity ImageJ. There are a total of 178 unique string variations extracted by the NER model that are mapped to the ImageJ software entity through disambiguation.

Table 16: Metadata Fields Statistics for the mentions linked to a repository. Synonyms retrieved through disambiguation that might link to the same entry are not counted

| Normalized metadata field | Count | %  |
|----------------------------|-------|----|
| package_url                | 149,015 | 100 |
| github_repo                | 143,834 | 96.52 |
| description                | 116,071 | 77.89 |
| homepage_url               | 36,306  | 24.36 |
| github_repo_license        | 39,464  | 26.48 |
| reference                  | 22,134  | 14.85 |
| RRID                       | 18,766  | 12.59 |
| other_urls                 | 18,766  | 12.59 |
| license                    | 13,485  | 9.04 |
This feature became available because we had the access to the structure of the papers, using their XML representation. Many other studies, for example, [24], process the text extracted from PDF, which does not show the structure. The current tendency of the publishers to keep the archival copies of the papers in the XML format is probably one of the best things that happened to the field of data mining from scholarly documents.

5.2. Software Name Variability in the Literature

The goal of building a comprehensive dataset of software mentions in the literature is to be able to assess software impact through informal citations. One of the main challenges is the variability under which a software can be mentioned, or ‘informally cited’ in a paper. Some of this variability is to be expected, such as differences between using the fullname or the acronym of a software (e.g., SPSS and Statistical Package for Social Sciences), authors using various software name variations (e.g., SPSS Statistics, IBM SPSS) or typos.

But probably the biggest string variability comes from how the NER model extracts software from text. For instance, the NER model might extract the following mentions: R package limma, limma R package, Limma, all pointing out to the same software.

Lastly, there is variability coming from typos that are occurring either due to the authors or because of XML parsing. If we want to truly get the impact of a particular piece of software, we need to be able to map all of these software naming variations to the same software entity.

5.3. Disambiguation

In order to map software variations to the same software entity, we built a software disambiguation model. We describe the model, based largely on string similarity algorithms and clustering techniques, under Section 2.4. Note that through this model, we are only able to disambiguate 28.88% mentions that constitute 78.18% of paper-software links. The other mentions either have no significant synonyms or are too ambiguous to disambiguate (Table 12). We propose this as a baseline model. Because the raw data is available, more sophisticated disambiguation algorithms can be employed. We want to note that the main challenge in disambiguating mentions in a dataset this large is the lack of labels, which means that the disambiguation tasks would have to be unsupervised. This poses challenges in terms of evaluation. We evaluated our disambiguation method using our biocuration team, which evaluated 5884 synonym pairs that we subsequently used to validate our model. The other challenge in using unsupervised methods, such as clustering, on a dataset this large, is the generation of distance matrices that would fit into working memory.

We also want to note that we experimented with using transformer-based models to generate embeddings for software mentions and compute similarity scores between pairs...
of strings by using the dot product or cosine similarity. We obtained unsatisfactory results creating similarity scores in this way. Pairs of strings that are semantically different than each other ended up having similar embeddings. This makes sense, as transformer-based models compute representational encodings for sequences based on context. It is possible that packages that are similar in some way, like `sklearn` and `scipy`, appear in similar contexts, and hence, will have similar embeddings. We hypothesize that the level of context around how a particular software is mentioned in a research paper is not granular enough to allow the computation of an embedding specific enough to differentiate that software from other similar, but different softwares. Basically, the language (and hence context) which authors use to mention `sklearn` is likely to be very similar to the language authors use to mention `scipy`. It makes sense that their embeddings will be close in n-dimensional space. We hypothesize that being able to use the context around a mention would, however, be useful for ambiguous cases when two different software can have the same name, or acronyms. This would be an interesting area of further work.

5.4. Use cases

As a philanthropic organization supporting and building technology to serve the computational needs of biomedical scientists, we rely on data on scientific software to inform our programmatic activities [46, 47] and technology strategy [48]. In this section we discuss a couple of ways the dataset has already been used in our work at the Chan Zuckerberg Initiative prior to the public release.

5.4.1. Trends in imaging

The Chan Zuckerberg Initiative considers imaging to be one of the key technologies in our effort to develop science and technologies to measure human biology in action [49, 50]. To fund this area more efficiently and support the relevant computational tools, we needed to understand the methods used in the field and the penetration of open source ones, in particular.

Modern biomedical imaging is significantly computational in nature. Thus we were able to use our data to identify the papers using various imaging software. We used publication data to get the time trends and the change of relative market share for both open and closed source imaging software.

5.4.2. Penetration of single-cell methods in biomedicine

Single-cell methods are another key area of biomedical technology supported by CZI [50]. To better focus our efforts, we needed data on the penetration of single-cell methods in the clinical research literature. The software used for analysis of single cell data is specific, so mention of this software in a paper can be a good marker of the usage of single cell methods. We were able to get a subset of papers that used single cell methods, and to estimate the penetration of these methods in the different biomedical subfields.

5.4.3. Other usage

We would like to note that the use cases mentioned in this section were also recognized by other people, for example, Wikidata Scholia project [51]. There are many other interesting questions, like the identifying the most influential authors, co-uses etc. [51]. We hope our dataset can be used by projects like Scholia and intend to integrate our results with Wikidata in the future releases.

6. Next Steps

We believe that there are a number of exciting questions this dataset can help answer. To start with, we can look into what the most used software is in a particular field (e.g. `neurodegeneration`, `single-cell biology`, `imaging`). We can go a step further and try to understand what the software is used for. Potential ideas include getting insights from paper or sentence topics, MESH terms, author-provided paper keywords, or information found in the sentence in which the software is being mentioned (note that we make this available). We can also start looking at differences between how software usage differs between particular fields, if any. Furthermore, we can explore measures of impact for software, whether those are number of informal citations (such as software mentions), or more sophisticated models. For instance, since we are now able to connect papers and software entities in an underlying graph, we can start exploring with graph-based models for impact. One particularly exciting idea would be to extend the notion of Eigenfactor, which has been proposed measure impact for journals and authors, to software. Other potential areas of further research include looking into open-access policies of most used or impactful software or exploring differences in how software usage varies over time. Last but not least, we can look into the impact of particular pieces of software and assess their impact.

The approach we took in this paper was to use an NER model to collect software string variations from a corpus of papers, and then disambiguate and link these mentions into clusters of software entities using DBSCAN [32] and a similarity matrix we built. Using this methodology, we were able to disambiguate about a third of the total number of unique mentions in our dataset, which covers about 78% of the total paper-software links. This means that we are losing information from the rest of the total number of mentions in our dataset. Future work can include improving the disambiguation algorithms to be able to cluster a larger percentage of our dataset under particular software entities.

For linking, we used an exact match search on a software mention in some of the most used software repositories, such as PyPI, CRAN, Bioconductor, SciCrunch and GitHub. We want to acknowledge that there are limitations in this approach. For instance, there can be different
software having the same acronyms, or different entities, whether software, databases, hardware or platforms with the same name. Moreover, in repositories that are not curated, such as GitHub, anyone can post a piece of software under whatever name they want. Being able to distinguish which is the true link for a piece of context would most likely require being able to look at the context in the text around a piece of software is being mentioned. Since we make the sentences in which a software mention appears available, we believe linking algorithms based on context are worth exploring. Improving the quality of linking software mentions to corresponding URLs in repositories or databases is an interesting area for further research.

7. Conclusion

We created one of the largest dataset of software mentions in the literature. For a subset of the data we used string similarity algorithms and unsupervised clustering techniques to disambiguate the software mentions into distinct software entities. We used a linking algorithm to connect the mentions to URLs in the PyPI, CRAN, Bioconductor indices and the SciCrunch and GitHub APIs. We make the dataset available to the community and believe there are a number of exciting next steps. It is our hope that this new resource helps foster new insights about software usage and impact in the literature.

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Appendix A. Schema Normalization

In this section, we offer more details about the process of normalizing schemas across the PyPI, CRAN and the Bioconductor indices, as well as the SciCrunch and GitHub APIs. By querying each of these repositories, we retrieve a number of metadata fields, which we map to a normalized set of fields (Table A.17).

Appendix B. Curation Guidelines

Background

A subset of 10,000 software mentions was curated by our domain experts, so as to identify the mentions that meet our definition of “Software” and exclude false positives. The curation process included two stages:

Stage 1: Curation of 1000 software mentions using five subcategories: Software, Algorithm, Database, Web Platform, Hardware (and “Other”).

During this first stage of labeling, we learned that it is hard to distinguish between Software and Algorithms as these terms are often used interchangeably by researchers. For the next labeling stage we considered them both as “Software”, whereas Database, Web Platforms and Hardware are considered as “Non-Software”.

Stage 2: Curation of 9000 software mentions using two main categories: Software and Not-Software.

This document outlines the definitions used for the annotation guidelines used by our domain experts for the manual labeling task, including examples of mentions to include (and exclude) in the dataset. The guidelines evolved through several iterative annotation cycles, taking into account feedback and suggestions from the curators where rules needed to be more explicit.

Definitions of subcategories

Our SciBERT model was trained on the Softcite Dataset [23]. We used their curation material as a baseline for our definitions:

Software includes all ‘obvious’ software: a good indication for inclusion is if a tool can be downloaded and installed; however, “Software as a Service”—platforms providing up-to-date cloud-based services for bioinformatic data analysis over a website—are also included in this category. Programming languages, such as “Java” or “R”, are annotated as “Software”; this includes mention of a script written in a language (the Softcite coding scheme explains that “programming languages are themselves software being used to create software”).

Algorithm is defined as a program, a problem-solving process that is computerized, or a function. The programs and algorithms may have implementations in different languages.

Database is a data collection or dataset, knowledgebase or repository. Note that in some cases, the database may be supported by a software framework (e.g. with the data made accessible via an interface); if the mention refers to the software component, it should be labeled as Software (often “Software as a service”).

Web platform includes web services such as “Facebook”, “Google”, or “Amazon”, or other online platforms that have a web interface.

Hardware is defined as physical instruments, devices, components or delivery systems, or other hardware (that may have software installed on it).

Curation—stage 1: How to annotate

Annotate each Software mention with one of the 5 categories:

- Software,
- Algorithm,
- Database,
- Web Platform,
- Hardware,

or with “Other” or “Unclear”.

1. For each Software mention 5 example sentences from papers are included. Use example sentences to understand the context and whether the mention is referred to as “software”, “version”, “program”, etc.

2. If the context is not clear, look online for more information, e.g. the About section of an online tool, information provided in a GitHub entry, a paper abstract describing the ‘mention’.

3. Where possible, label the mention with one of the subcategories. Mentions that don’t fit any of the subcategories 1-5 should be labeled with “Other” (see examples below).

4. For mentions where more than one subcategory applies, use the following rules:

   - Where the distinction between “Software” and “Algorithm” is difficult → select “Software”.
   - Where the mention could be “Software” and another category → select “Software”.
   - Similarly, where it could “Algorithm” and another category → select “Algorithm”. For example, “VISTA is a comprehensive suite of programs and databases for comparative analysis of genomic sequences” → label as “Algorithm”.

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Table A.17: Schema Normalization. Mappings between Normalized fields and corresponding fields from each resource: PyPI, CRAN, Bioconductor, SciCrunch API, GitHub API

| Normalized Field | PyPI       | CRAN       | Bioconductor | SciCrunch API | GitHub API |
|------------------|------------|------------|--------------|---------------|------------|
| mapped_to        | PyPI package | CRAN Package | Bioconductor Package | Resource Name | best.github_match |
| source           | PyPI Index | CRAN Index | Bioconductor Index | SciCrunch API | GitHub API |
| package_url      | PyPI pypi_url | CRAN pypi_url | Bioconductor pypi_url | SciCrunch pypi_url | GitHub pypi_url |
| description      | query pypi_url page | query CRAN Link | query Bioconductor Link | Resource Name | github_url |
| homepage_url     | query pypi_url page | query CRAN Link | query Bioconductor Link | Resource Name | github_url |
| other_urls       | None | None | None | Alternate URLs + Old URLs | None |
| github_repo      | query pypi_url page | query CRAN Link | query Bioconductor Link | SciCrunch API | github_url |
| github_repo_license | None | None | None | None | github_repo_license |
| reference        | None | query CRAN Link | query Bioconductor Link | Reference Link or Proper Citation | GitHub API |
| RRID             | None | None | None | Resource ID | None |
| scicrunch_synonyms | None | None | None | synonyms | None |
Where the mention could be labeled with two other categories → select either. (Accuracy was deemed less important here as the final goal was to distinguish between Software+algorithm vs not-Software).

5. For ambiguous mentions and acronyms, where the example sentences appear to refer to multiple different things, select “Unclear”.

Curation—stage 2: How to annotate
Annotate each Software mention with one of the two main categories:
• Software & Algorithm,
• Not Software (including databases, web platforms, hardware, or Other) Or with “Unclear”

How to annotate:
1. As before, use example sentences to understand the context and whether a mention is about “software”, “program”, “algorithm” etc. If the context is not clear from the examples, look online for an online tool, a GitHub entry, a paper abstract, etc.
2. For ambiguous mentions, where the sample sentences appear to refer to multiple different things and don’t fall clearly into one of two main categories, select “Unclear”.
3. True software mention that appear as partial terms should be labeled as Software. For example, the Software mention “Random” can be labeled as Software if the example sentences clearly refer to the same software (“The superior accuracy of activity measures was confirmed using Random Forest and predictive modeling techniques”).

Examples
Examples of tools that should be labeled as “Software & Algorithm” (Curation stage 2) are shown in Table B.18.
Examples of tools that should be labeled as “Not-Software” (Curation stage 2) are shown in Table B.19. The different types (subcategories) used for labeling in stage 1 are indicated in the last column.
Examples of mentions that don’t fit into the five subcategories are listed in Table B.20. They should be labeled as “Not-Software” in Curation stage 2 (or as “Other” in stage 1).

Appendix C. Datasets Description
In this section, we provide details about the datasets we make available.

There are six directories: raw, disambiguated, linked, evaluation and intermediate. Files with the extension tsv are tab separated, files with the extension csv are comma separated, files with the suffix pkl are Python serialized objects [52], files with the suffix gz are gzipped. Note that tab separated files may contain embedded quotes, which do not have special meaning, while in comma separated files they do according to the usual conventions.

Appendix C.1. Raw files
The raw directory contains extracted mentions before disambiguation and linking. It has the following three files: comm_raw.tsv.gz (PMC OA commercial subset), non_comm_raw.tsv.gz (PMC OA non-commercial subset), and publishers_collection_raw.tsv.gz (CZ Publishers’ collection). Each file also contains a curation_label field to denote the curation label our curation team gave to each software entry.

The files comm_raw.tsv.gz (commercial subset) and non_comm_raw.tsv.gz (non-commercial subset) are tab separated, gzipped, and have the following fields:
license either comm or non_comm,
location the location of the file from which the mentions are extracted, for example, comm/Micropl/PMC8475362.nxml,
pmcid PMC id of the paper (with the prefix “PMC” stripped),
pmid PubMed id of the paper,
doi DOI of the paper,
pubdate publication year according to the metadata in the paper source,
source part of the paper from which the mention was extracted; this is either a section in the main text of the paper (like ”introduction” or ”materials and methods”) or another part of the paper: paper_title, paper_abstract, tab_caption, fig_caption.
number sequence number of the object, from which the mention was extracted:
• for body text, paragraph number;
• for figure and table captions, the number of the figure or table;
• otherwise, zero,
text the sentence, from which the software mention was extracted,
software the extracted software mention,
version the extracted software version,
ID software mention ID.
curation_label curation result for the software mention:
• software if the mention was labeled as software by the curation team.
Table B.18: Curation Guidelines - Examples of mentions: software & algorithm. These examples were used for training our curation team.

| Software mention ID | Software mention | Link | Description at the link and notes |
|---------------------|------------------|------|----------------------------------|
| SM2407              | ABAQUS           | https://en.wikipedia.org/wiki/Abaqus | “Abaqus FEA (formerly ABAQUS) is a software suite for finite element analysis and computer-aided engineering” |
| SM6358              | gplots           | https://cran.r-project.org/web/packages/gplots/index.html | “Various R programming tools for plotting data” |
| SM5899              | Java             |       |                                   |
| SM1591              | Perl             |       |                                   |
| SM8176              | Keras            | https://keras.io/ | “Keras is an open-source software library that provides a Python interface for artificial neural networks” |
| SM1028              | I-TASSER         | https://zhanggroup.org/I-TASSER/ | “server for protein structure and function prediction” |
| SM1500              | GEPIA            | http://gepia.cancer-pku.cn/ | “interactive web server for analyzing the RNA sequencing expression data” |
| SM534               | InterProScan     | https://www.ebi.ac.uk/interpro/about/interproscan/ | “InterProScan is the software package that allows sequences to be scanned against InterPro’s member database signatures.” |
| SM14721             | SurveyMonkey     | https://www.surveymonkey.co.uk/ | online questionnaire tool |
| SM1693              | ARB              | https://en.wikipedia.org/wiki/ARB_Project | “The ARB Project is a free software package for phylogenetic analysis of rRNA” |
| SM6650              | BiNGO            | https://www.psb.ugent.be/cbd/papers/BiNGO/Home.html | “a Java-based tool to determine which Gene Ontology (GO) categories are statistically overrepresented in a set of genes or a subgraph of a biological network” |
| SM24091             | ADMIXTURE        | https://bioinformaticshome.com/tools/descriptions/ADMIXTURE.html | “Enhancements to the ADMIXTURE algorithm for individual ancestry estimation.” |
| SM34896             | ABySS            | https://rcc.fsu.edu/software/abyss | “ABySS is a Bioinformatics program designed to assemble genomes from small paired-end sequence reads” |
| SM8175              | Adam             | https://towardsdatascience.com/adam-latest-trends-in-deep-learning-optimization-6be9a291375c | “Adam is a replacement optimization algorithm for stochastic gradient descent for training deep learning models” |
| SM6044              | Blast            | https://blast.ncbi.nlm.nih.gov/Blast.cgi | “BLAST is an algorithm and program for comparing primary biological sequence information” |
| SM15716             | bowtie           | https://bio.tools/bowtie2 | “Bowtie 2 is an ultrafast and memory-efficient tool for aligning sequencing reads to long reference sequences” |
| SM1735              | TopHat           | https://ccb.jhu.edu/software/tophat/index.shtml | “TopHat-Fusion algorithm” |
| SM4671              | MySQL            | https://en.wikipedia.org/wiki/MySQL | open-source relational database management system |
| SM3262              | ClueGO           | https://apps.cytoscape.org/apps/cluego | Software plugin |
| SM4915              | R script         |       | Software script API |
| SM5658              | CUDA             | https://docs.nvidia.com/cuda/ | software that has the same name as the company that develops it |
| SM517               | DNASTAR          | https://www.dnastar.com/ | software that has the same name as the output format (if mention is clearly the software) |
| SM1004              | FASTA            | https://en.wikipedia.org/wiki/FASTA_format | |

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Table B.19: Curation Guidelines - Examples of mentions: not-software. These examples were used for training our curation team.

| Software mention ID | Software mention | Link | Description at the link and notes | Subcategory |
|---------------------|------------------|------|-----------------------------------|-------------|
| SM37528             | WorldClim        | https://www.worldclim.org/data/v1.4/worldclim14.html | “Maps, graphs, tables, and data of the global climate” | Database    |
| SM15080             | ArrayExpress     | https://www.ebi.ac.uk/arrayexpress/ | Data archive | Database    |
| SM8406              | cgMLST           | https://www.cgmlst.org/ncs | “Nomenclature Server” | Database    |
| SM15100             | ClinVar          | https://www.ncbi.nlm.nih.gov/clinvar/ | “ClinVar aggregates information about genomic variation” | Database    |
| SM2352              | GitHub           | https://github.com/ | Software repository | Database    |
| SM3888              | Facebook         | | “online social media and social networking service” | Web platform |
| SM5608              | Google Earth     | https://play.google.com/about/howplayworks/ | “Google Earth is a geobrowser” | Web platform |
| SM5472              | Google Play      | https://en.wikipedia.org/wiki/Kinect | “Kinect is a line of motion sensing input devices produced by Microsoft” | Hardware    |
| SM5379              | ActiGraph        | https://actigraphcorp.com/ | “ActiGraph’s wearable accelerometer-based biosensors” | Hardware    |
| SM3147              | Leica            | https://leica-camera.com/en-GB | Company name and product name | Hardware    |
| SM5200              | Kinect           | https://en.wikipedia.org/wiki/Kinect | | Hardware    |

- **not_software** if labeled as not-software by the curation team
- **unclear** if a call could not be made based on available information
- **not_curated** if mention has not been curated.

Results of extraction from the CZ Publishers’ collection are in the file *publishers_collection.tsv.tgz*. It is a tab separated gzipped file with the following fields:

- **doi** paper DOI,
- **pubdate** publication year, according to the metadata in the paper source,
- **source** part of the paper from which the mention was extracted; this is either a section in the main text of the paper (like “introduction” or “materials and methods”) or another part of the paper: **paper_title**, **paper_abstract**, **tab_caption**, **fig_caption**.
- **number** sequence number of the object, from which the mention was extracted:
  - for body text, paragraph number;
  - for figure and table captions, the number of the figure or table;
  - otherwise, zero,

- **text** the sentence, from which the software mention was extracted,
- **software** the extracted software mention.
- **ID** software mention ID.
- **curation_label** curation result for the software mention:
  - **software** if the mention was labeled as software by the curation team
  - **not_software** if labeled as not-software by the curation team
  - **unclear** if a call could not be made based on available information
  - **not_curated** if mention has not been curated.

**Appendix C.2. Disambiguation Results**

The linked directory contains the directory *synonyms_files* and the files *comm_disambiguated.tsv.gz*.

The *synonyms_files* directory contains synonyms dictionaries used in the disambiguation process, stored in the pickle format. The following files are available:

- **pypi_synonyms.pkl** Python dictionary mapping from a pypi package and an array of synonyms generated through the Keywords Synonym Generation process 2.4.1
Table B.20: Curation Guidelines - Examples of mentions: “other” mentions. These examples were used for training our curation team.

| Software mention ID | Software mention | Link                                                                 | Description at the link                                                                 | Notes                          |
|---------------------|------------------|----------------------------------------------------------------------|------------------------------------------------------------------------------------------|--------------------------------|
| SM5111              | ANOSIM           | [https://www.nhm.uio.no/english/research/infrastructure/past/help/anosim.html](https://www.nhm.uio.no/english/research/infrastructure/past/help/anosim.html) | ANOSIM (ANalysis Of Similarities) is a non-parametric test of significant difference.     | Statistical test               |
| SM1779              | LOESS            | [https://www.statsdirect.com/help/nonparametric_methods/loess.htm](https://www.statsdirect.com/help/nonparametric_methods/loess.htm) | Method for fitting a smooth curve between two variables.                                   | Statistical test               |
| SM5147              | ENCODE           | [https://www.encodeproject.org/](https://www.encodeproject.org/)        | Public research project which aims to identify functional elements in the human genome.    | Consortium/project             |
| SM1166              | R Core           | [https://www.r-project.org/contributors.html](https://www.r-project.org/contributors.html) | A core group, the R Core Team, with write access to the R source                          | Group of people                |
| SM1901              | R Foundation for Statistical Computing | [https://www.r-project.org/foundation/](https://www.r-project.org/foundation/) | The R Foundation is a not for profit organization.                                       | Group of people                |
| SM3954              | RE-AIM           | [https://re-aim.org/](https://re-aim.org/)                              | RE-AIM is a framework to guide the planning and evaluation of programs according to the 5 key RE-AIM outcomes: Reach, Effectiveness, Adoption, Implementation, and Maintenance. | Project                        |
| SM5429              | iOS              | [https://www.thermofisher.com/uk/en/home/life-science/microarray-analysis/affymetrix.html](https://www.thermofisher.com/uk/en/home/life-science/microarray-analysis/affymetrix.html) | “Affymetrix microarray solutions include necessary components for a microarray experiment, from arrays and reagents to instruments and software” | Operating system               |
| SM6157              | Affymetrix       | [https://www.thermofisher.com/uk/en/home/life-science/microarray-analysis/affymetrix.html](https://www.thermofisher.com/uk/en/home/life-science/microarray-analysis/affymetrix.html) | “Affymetrix microarray solutions include necessary components for a microarray experiment, from arrays and reagents to instruments and software” | System with multiple components, including software |
| SM16352             | nCounter         | [https://nanostream.com/products/ncounter-analysis-system/ncounter-pro/](https://nanostream.com/products/ncounter-analysis-system/ncounter-pro/) | “Applications such as targeted re-sequencing, metagenomics, small genome sequencing, targeted gene expression profiling” | System with multiple components, including software |
| SM3461              | Arduino          | [https://www.arduino.cc/](https://www.arduino.cc/)                      | “Applications such as targeted re-sequencing, metagenomics, small genome sequencing, targeted gene expression profiling” | System with multiple components, including software |
| SM1127              | MiSeq            | [https://emea.illumina.com/systems/sequencing-platforms/miseq.html](https://emea.illumina.com/systems/sequencing-platforms/miseq.html) | “Applications such as targeted re-sequencing, metagenomics, small genome sequencing, targeted gene expression profiling” | System with multiple components, including software |
| SM8468              | Apache           | [https://www.apache.org/licenses/LICENSE-2.0](https://www.apache.org/licenses/LICENSE-2.0) | A quality assessment tool for diagnostic accuracy studies                                 | License                        |
| SM338               | QUADAS           | [https://www.bristol.ac.uk/population-health-sciences/projects/quadas/quadas-2/](https://www.bristol.ac.uk/population-health-sciences/projects/quadas/quadas-2/) | A quality assessment tool for diagnostic accuracy studies                                 | Tools that are checklists      |
| SM1908              | RNAseq           |                                                                      | Sequencing technique                                                                    | Method                          |
| SM5014              | SOLiD            |                                                                      | SOLiD next-generation sequencing technology                                              | Method                          |
cran_synonyms.pkl Python dictionary mapping from a CRAN package and an array of synonyms generated through the Keywords Synonym Generation process 2.4.1

bioconductor_synonyms.pkl Python dictionary mapping from a Bioconductor package and an array of synonyms generated through the Keywords Synonym Generation process 2.4.1

scicrunch_synonyms.pkl Python dictionary mapping from a mention found in SciCrunch and its synonyms retrieved through the SciCrunch API 2.4.2

extra_scicrunch_synonyms.pkl Python dictionary mapping from a mention found in SciCrunch and its synonyms retrieved by parsing the corresponding URL in SciCrunch 2.4.2

string_similarity_synonyms.pkl Python dictionary mapping from a mention found in the comm_IDs.tsv.gz corpus and its synonyms retrieved through the Jaro Winkler algorithm, together with the corresponding confidences 2.4.3. Only pairs of synonyms with a similarity confidence of $\geq 0.9$ are kept. The file has the following format:

- software_mention - mention synonyms are computed for
- ([synonyms], [synonyms_confidences]) - tuple containing two arrays:
  - synonyms: list of synonyms for software mention
  - synonyms_confidences: Jaro Winkler similarity scores between synonyms and software mention, as given by the textdistance python package [38]

synonyms.tsv.gz tab separated, gzipped comma file used as input for the clustering algorithm, after post-processing. The file is built by combining information from files pypi_synonyms.pkl, cran_synonyms.pkl, bioconductor_synonyms.pkl, scicrunch_synonyms.pkl, extra_scicrunch_synonyms.pkl, and string_similarity_synonyms.pkl, and performing additional clean-up. The file has the following format:

- ID ID for software_mention,
- synonym_ID ID for synonym,
- software_mention software_mention to compute synonyms for
- synonym a synonym for software_mention
- synonym_conf confidence for this synonym pair (as described in 1)
- synonym_source source for this synonym pair:
  - SciCrunch if synonym pair retrieved from scicrunch_synonyms.pkl
  - extra_scicrunch_synonyms.pkl
  - Bioconductor if synonym pair retrieved from bioconductor_synonyms.pkl
  - CRAN if synonym pair retrieved from cran_synonyms.pkl
  - PyPI if synonym pair retrieved from pypi_synonyms.pkl
  - string_similarity if synonym pair retrieved from string_similarity_synonyms.pkl

Appendix C.2.1. Disambiguated File

The comm_disambiguated.tsv.gz file is a tab separated, gzipped file corresponding to the disambiguation results for comm.tsv.gz. The file was obtained by running the DBSCAN-based clustering algorithm on synonyms.csv as described in 2. The file has all the fields in comm.tsv.gz with the additional fields:

- mapped_to_software software entity (or cluster) the software mention described in this entry is predicted to be part of; For example, for the software mention ‘R package limma’, the mapped_to_software might be ‘limma’.

- mapped_to_software_ID ID of mapped_to_software

Appendix C.3. Linking Results

The linked directory contains the following directories: normalized and raw and the file metadata.tsv.gz.

Appendix C.3.1. Raw Metadata Files

The raw directory contains raw metadata files obtained by querying the PyPI, CRAN, Bioconductor, SciCrunch and GitHub APIs on mentions extracted by the NER algorithm from the comm.tsv.gz corpus (PMC-OA commercial subset). The directory contains the following comma separated files:

- bioconductor_raw_df.csv raw metadata file obtained by querying Bioconductor on mentions extracted from the comm.tsv.gz. Has fields:
  - Bioconductor Package
  - Bioconductor Link
  - Maintainer
  - Title

- cran_raw_df.csv raw metadata file obtained by querying CRAN on mentions extracted from the comm.tsv.gz. Has fields:
  - CRAN Package
  - CRAN Link
  - Title
github_raw_df.csv raw metadata file obtained by querying GitHub on mentions extracted from the comm.tsv.gz. Has fields:

- software_mention
- best_github_match
- description
- github_url
- license
- exact_match

pypi_raw_df.csv raw metadata file obtained by querying PyPI on mentions extracted from the comm.tsv.gz. Has fields:

- pypi_package
- pypi_url

scicrunch_raw_df.csv raw metadata file obtained by querying SciCrunch on mentions extracted from the comm.tsv.gz. Has fields:

- software_name
- scicrunch_synonyms
- Resource Name
- Resource Name Link
- Description
- Keywords
- Resource ID
- Resource ID Link
- Proper Citation
- Parent Organization
- Parent Organization Link
- Related Condition
- Funding Agency
- Relation
- Reference
- Website Status
- Alternate IDs
- Alternate URLs
- Old URLs
- Reference Link

Appendix C.3.2. Normalized Metadata Files

The normalized directory contains normalized versions of the raw metadata files. Files are normalized to a common schema as described in A.17. The directory contains the following comma separated files:

bioconductor_df.csv normalized metadata file obtained by querying Bioconductor on mentions extracted from the comm.tsv.gz,

cran_df.csv normalized metadata file obtained by querying CRAN on mentions extracted from the comm.tsv.gz,

github_df.csv normalized metadata file obtained by querying GitHub on mentions extracted from the comm.tsv.gz,

pypi_df.csv normalized metadata file obtained by querying PyPI on mentions extracted from the comm.tsv.gz,

scicrunch_df.csv normalized metadata file obtained by querying SciCrunch on mentions extracted from the comm.tsv.gz

Appendix C.3.3. Master Metadata File

The metadata.tsv.gz file is a concatenation of all the metadata files in the normalized directory. Each file in the normalized directory, as well as the metadata.tsv.gz file has the following fields:

ID a unique identification for each software,

software_mention the canonical string for the given software mention,

mapped_to list of values to which the software was mapped,

source mapping source (PyPI, CRAN, SciCrunch, GitHub, Bioconductor),

platform list of platforms for the given software,

package_url URL for the given package,

description list of descriptions associated with software in the databases,

homepage_url list of homepages for the software,

other_urls list of other URLs for the given software mined from the database,

license list of licenses under which the software is released,

github_repo list of GitHub repositories for the software,

github_repo_licenses list of licenses listed on the GitHub repositories,

exact_match True if an exact string match was found for the given software mention, False if a fuzzy match was used instead,

RRID RRID for the software retrieved from SciCrunch [42],

reference journal articles linked to the software, identified by DOI, PMID or RRID,

scicrunch_synonyms synonyms for software according to SciCrunch [42].
Appendix C.4. Evaluation Files

The directory evaluation contains files used for cura-
tion and evaluation.

Appendix C.4.1. Curated Software Mentions

The file curation_top1k_mentions_multi_labels.csv.gz contains the results of curation of top 10,000 mentions over five categories. It is a comma separated file with the following fields:

ID unique identifier for software mention,
software_mention name of software mention,
text five example sentences from articles where the software mention appears,
multi_label manually curated label selected for the software mention. Possible labels: software, algorithm, database, hardware, web platform, other, unclear,
label manually curated label selected for the software mention. Possible labels: software&algorithm, not-software, unclear,
Curation_comments curator’s explanation why a specific label was chosen, including links to online tools, spelled-out acronyms, information found through online searches and/or in example sentences.

The file curation_top10k_mentions_binary_labels.csv.gz contains the results of curation of top 1000 mentions over two categories. It is a comma separated file with the following fields:

ID unique identifier for software mention,
software_mention name of software mention,
text five example sentences from articles where the software mention appears,
label manually assigned label by the curators:
• correct if the package_url generated for software_mention is correct;
• incorrect if the package_url generated for software_mention is incorrect;
• unclear if there isn’t enough information to assess whether or not the package_url generated for software_mention is correct;

The file evaluation_disambiguation.csv.gz presents the manual evaluation of disambiguation. Curators were tasked with assessing if a pair of string software mentions are synonyms. The file is a gzipped comma-separated file with the following fields:

link_label name of software mention,
synonym synonym generated by the disambiguation algorithm,
text five example sentences from articles where the synonym mention appears,
label manually curated label selected for the software mention, synonym pair. Possible labels: 'Exact', 'Narrow', 'Not software', 'Unclear', 'Not synonym'
curation_notes curators’ explanation why a specific label was chosen.

Appendix C.4.2. Linking & Disambiguation Evaluation Files

The file evaluation_linking.csv.gz presents the manual evaluation of linking. Curators were tasked with assessing if the link generated for a particular software_mention was correct. The file is a gzipped comma-separated file with the same fields as comm_curated.tsv.gz and metadata.tsv.gz above, and an additional field:

software_mention manually assigned label by the curators:

Appendix C.5. Intermediate Files

The directory intermediate_files contains the following files: mention2ID.pkl and freq_dict.pkl.

The file mention2ID.pkl is a mention to ID mapping connecting all the plain text software mentions extracted by the NER algorithm from the comm_raw.tsv.gz, non_comm_raw.tsv.gz and publishers_collection_raw.tsv.gz to a unique ID. The file is in the pickle format and the data is stored as a Python dictionary. The keys are plain-text software mentions across all three datasets, and the values are unique IDs across all three corpora.
The file `freq_dict.pkl` is a **mention to frequency** mapping connecting all plain text software mentions extracted by the NER algorithm from the `comm_raw.tsv.gz` to their frequency on the `comm_raw.tsv.gz` dataset. We define frequency as the total number of unique papers a mention appears in the PMC-OA *comm* dataset. The file is in the pickle format and the data is stored as a Python dictionary. The keys are plain-text software mentions in `comm_raw.tsv.gz`, and the values are the corresponding frequencies.

**Appendix D. Additional Examples of String Variability**

Additional examples of string variability can be found on Figures D.8 and D.9.
matrix laboratory
MATLAB
MATLAB, Signal Processing Toolbox and Statistics Toolbox
MATLAB
MATLAB
MATLAB
MatLab
MatLab
MatLab
Matlab
Matlab
MATLAB, Statistics and Machine Learning Toolbox
mATLab)
Matlab)
matlab
matlab - the language of technical computing
matlab)
matlab, signal processing toolbox and statistics toolbox
matlab, statistics and machine learning toolbox
MATLAB
matrix laboratory
matlab
MATLAB - The Language of Technical Computing
MATLAB BGL
MATLAB IDE
MATLAB HMM
MATLAB GUI
MATLAB GPU
MATLAB FDA
MATLAB EFD
MATLAB DIC
MATLAB DGN
MATLAB CVX
MATLAB CPU
MATLAB App
MATLAB® SVM
MATLAB ANN

Figure D.8: Examples of string variability for the software ‘MATLAB’ (http://www.mathworks.com/products/matlab/), as extracted by the NER model from the PMC-OA corpus

graphpad, prism
GraphPad
GraphPAD
GraphPAD
GraphPad
GraphPad)
GRAPHPAD
graphpad
graphpad)
GraphPad, Prism
GraphPad, Prism
GraphPad- Prism
GraphPad-InSTAT
GraphPad-InStat
GraphPad-Instat
GraphPad-Prism4
GraphPad-Prism8
GraphPad-Prism7
GraphPad-Prism©
GraphPad-prism5
GraphPad “Prism
GraphPad-prism7
GraphPad-Prism5
GraphPad “PRISM
GraphPad prism8
GraphPad ©Prism
GraphPad prism®
GraphPad prism
GraphPad prism9
GraphPad.PRISM®
GraphPad prism7
GraphPad prism6
GraphPad prism5
GraphPad prism4
GraphPad prism3
GraphPad primer
GraphPad instat
GraphPad)

Figure D.9: Examples of string variability for the software ‘GraphPad’ (http://graphpad.com/), as extracted by the NER model from the PMC-OA corpus