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# Introduction

Today’s scientific research relies on a use as well as production of various types of research artifacts, a.k.a. research resources, ranging from digital to physical {schindler2019annotation}. One of key digital research artifacts, broadly used in a scientific investigations, is software. Many scientists *use* already existing software for various purposes during their research as well as *create* a new software as part of their research work {goble2014better , hannay2009scientists }.

Almost every software has information associated with it which can be extracted. Version, name of developer, license, abbreviation, URL, citation, release, extension, etc. are among the most obvious examples.

However there are also other kinds of information about a software that is non-obvious and challenging to extract. For example, in a given line of text in a research paper a software can be mentioned to indicate weather a researcher is using a software for a particular purpose, introducing a novel software, providing repository information about the deposition of the software, or just mentioning the name of the software. In addition information about category of a software: such as application, plugin, programming environment, operating system, etc. can also be concealed in a textual description in a scientific paper {schindler2021somesci}.

Extraction of all such variations of information about software from the scientific publications has critical importance. This is because, information about a software can be used to uniquely identify each software and avoid ambiguity regarding which software or version a researchers have used in their literature. Being able to uniquely identify a software with its specification is also advantageous to guarantee reproducibility of research results as well as providing clear understanding how results of research have been produced {kruger2019literature}. In addition, knowledge about a software mention type or purpose of use can help to determine which set of software artifacts can be suitable for a given study or to compare results obtained from various software in a given study. Furthermore, knowledge about software use and purpose of use in the literature, supports semantic analysis and retrieval of scientific publications based on use of particular software {schindler2019annotation}.

Even though software citation principles have been already established by a scientific community {callaghan2014joint, smith2016software}, software citation practice in reality is still informal and incomplete {schindler2021somesci}. This makes it difficult to extract information about software that would help to attribute credits to the creators of software, reproduce research results, disambiguate one software from another, etc.

Various manual and rule based techniques has been attempted in the past to extract information about software. However, machine learning based techniques have not been exploited despite being more powerful. The main reason was lack of training data which can support training of a classifier for software information extraction {schindler2021somesci}. Producing reliable ground truth data could be accomplished by crowd sourcing for general domains but it is expensive particularly for domain-specific and scientific publications as it requires expert domain knowledge {beltagy2019scibert}. Fortunately, identification of software mentions from scientific articles has drawn more attention over the past years and now various labelled data sets, such as BioNerDs {duck2013bionerds} , SoftCite {du2021softcite}, are available. Recently a more comprehensive data set, SoMeSci, has been published. SoMeSci contains high quality manually annotated data sets that cover broader range of information about software paving a way for a use of machine learning based approach for the automatic extraction of information about software {schindler2021somesci}.

## Scope

This thesis work tries to apply machine learning technique using SoMeSci data set to extract information about software mentions, particularly, to identify for what purpose a software is used in a given context of text.

To accomplish this, first possible list of software usage purposes have been identified via extensive analysis of literature and other sources like software ontologies and repositories. Then already existing annotations of software usage mentions in the SoMeSci data set has been extended with software purpose labels.

Once software usage mentions in the SoMeSci data set has been labelled with software purpose labels, the data set has been cleaned, analyzed, transformed, and used for classification purpose.

## Objectives of the research

The main objectives to be accomplished in this thesis work are:

* To perform literature review on the importance of software in a research.
* To carry out analysis of literature and software ontologies to identify main types of purposes of software use in a research.
* To extend SoMeSci data set with software usage purpose annotation.
* To perform analysis of SoMeSci data set to drive interesting facts about the data set.
* To select a suitable feature, classifier, and to train a classifier model.
* To evaluate and optimize results.

## Overview of the report

Chapter 1 makes a soft introduction about why it is important to extract information about software, specifies scope and objective of the thesis.

Chapter 2 focuses on highlighting the role of software in a research to indicate driving information about software used in a research is an important task.

Chapter 3 focuses to identify possible types of software usage purposes from literature and software ontology. This is an important step taken to extend software usage statements in the SoMeSci data set with software purpose annotations.

Chapter 4 is about the data set. It explains how SoMeSci data set has been extended with software purpose annotations, annotation tool used, and the annotation process. In addition explains about data pre-processing, transformation to suitable format and splitting for classification on purpose. At the end, results of analysis of the extended SoMeSci data set has been presented.

Chapter 5 discusses and compares a various models suitable for classification of software purpose from a text.

Chapter 6 focuses model training , optimization and evaluation of various scenarios.

Chapter 7 discusses about classification and results of the evaluation.

Chapter 8 summarizes results and provides conclusion.

## Summary

This chapter has presented a gentle introduction into types of information associated with software artifacts, extraction approaches and why it is important to extract information about software. The data set to be used, scope and goal of the work has also been discussed.

The next chapter presents the role of software in a modern research to give more elaborate understanding about the impact of software in a scientific investigations indicating why it is worth to extract knowledge about software.

# The role of Software in Scientific research

## Introduction

Nowadays scientific research is unthinkable without a use of software and investigations in various areas of science are becoming increasingly reliant on software tools {goble2014better, storer2017bridging, hannay2009scientists, jimenez2017four}.

A software is very important asset for building a scientific knowledge and more discoveries in a research are made possible than ever by a use of software tools that automate processing of huge amount of data {jimenez2017four}. Typically a software is used in a research for data processing tasks such as data analysis, modeling, simulation, control processes, knowledge dissemination, etc. {hannay2009scientists, pan2016disciplinary}.

In modern research, a scientific software is as important as any lab-equipment {wilson2014best}. However, the development of scientific software is much more complicated and fundamentally different from an ordinary commercial software like accounting software. Scientific software requires specialized domain knowledge for its development and requires a direct involvement of domain expert or scientist {wilson2014best, segal2008developing}. Due to this, an increasing number of scientists are developing a software as part of their research work or directly taking part in the development process of a research software {jimenez2017four, kanewala2014testing}.

According to surveys conducted in the UK and USA, 2008 and 2017 respectively, most scientists agree that software plays an important role in their research work {hettrick2014uk, nangia2017track}. Participants of the survey, in UK, were 2000 researchers working in various areas of science in roles ranging from student to senior academic staff whereas participants of the survey, in USA, were members of the US National Postdoctoral Association.

The results from of UK survey {hettrick2014uk} indicate that :

* 38% of researchers spend at least 20% of their time developing a software.
* Almost half of scientists spend more time creating software as part of their research work than five years ago .
* Over 50% of survey respondents reported that they develop their own software.
* Nearly 70% claim that their research directly depends on use of a software &
* Over 90% of scientists say software is important for their research.

The results from of USA survey {nangia2017track} indicate that:

* Over 90% of scientists use software.
* 63% of respondents state that their research is impossible with out using software.
* 31% of scientists say that they could do their work without using a software but more effort would require.
* Only 6% of survey respondents say that there would be no significant difference in their task if they do not use software.

Overall, results from the two surveys clearly indicate that software is pervasive in scientific investigations and many researchers use as well as develop a software for their research.

Even though software plays an important role in a modern research, usually the contributions of software is understated. This can be seen from the poor citation practice of software in research papers across several fields of research {schindler2021somesci,yang2018important, pan2016disciplinary}. In an attempt to promote the recognition of the roles of scientific software in a research, the ReSA has collected literatures that evident the roles software play in a research, at Zetoro group library. The main aim of ReSA is to influences decision makers to acknowledge contributions of a research software and give credits to its developers.

The next section presents more details about the role of software: in general, in specific domains, and in research breakthroughs.

## General roles of software in a research

Software is playing crucial roles in a research and making a shift in a research culture in terms of enabling automation of analysis pipelines, creation of new ways of analysis via computational models, supporting sophisticated analysis of large volume of data, documentation of a research, etc. {jay2020software}.

Some of the most general roles of a software in a research are:

* *A software dictates the quality of a research outcome* {hannay2009scientists}. Outcome of a research becomes unreliable or even useless if there is an error in the software {soergel2014rampant}. For example, several scientists retracted their scientific publications up on a retrospective discovery of a bug in their software {wilson2014best,merali2010computational,miller2006scientist}. A more palpable failure of a research ambition due to an error in the software, for instance, is the failure of *Ariane rocket* in 1996 {enwiki:1054482061}.
* Software helps to explore und understand a research problem {hannay2009scientists}.
* Results from a scientific software is presented as an evidence to support a research conclusion {kanewala2014testing}.
* A software also helps to document a research process and to *validate results of a given research* {jay2020software}. Executable cells in a Jupyter notebook is one real world example where a software can be used to validate a research result.
* Software allows experiments to be made beyond constrains of the physical world. This is because experiments that run on a computer are not limited by processes that occur in nature but only by the laws imbedded in the computer code {wolfram1984computer}.

## Domain specific examples

A software is being extensively used for a research in various areas of science such as physics, chemistry, space science, life science and so on.

The physics research facility, the Large Hydron Collider at CERN, for instance uses a software with more than 5 million lines of code which is used for processing of terabytes of data generated from experiments {storer2017bridging}.

In a nuclear research, a software is being developed increasingly to be used for experiments {yan2017case}. For example, testing a modification in a nuclear weapon can not be done on a field, but instead a software that simulate the impact of modification is usually used {kanewala2014testing}. This is because testing of a nuclear weapon on a field is banned by regulations like nuclear test ban treaties (NTBT) in addition to the potential disaster that testing a nuclear weapon poses to the environment and life {enwiki:1053274189}.

In chemistry research, a software can be used to model and simulate chemical processes that are challenging, too complex or expensive to conduct in reality. Karplus and Levitt used computer simulations for their joint-research “the development of multi-scale models for complex chemical systems” and won a Nobel prize in 2013 for their work {storer2017bridging, andre2014nobel}.

In a climate and environmental studies, software is used to make predictions about climate changes. For example historical temperature data can be integrated to make predictions about future temperature variations {storer2017bridging}.

In a space science, space probes heavily rely on software. In this case a software helps navigate space crafts to other planets, processes and transmits scientific data back to Earth for further processing, helps researchers interpret results, etc.{lutz2011software}.

In medical research and diagnosis, imaging software plays a critical role to assist medical researchers, for instance, for early isolation of cancer cells. The main reason for low chance of survival from cancer is mainly due to late detection of cancer cells in the body. This makes a diagnosis of cancer to be a time critical task and early identification of cancer implies curability of a disease and a higher chance of survival {wagner2004challenges}. Especially on the early stages, it is not straight forward to determine which cells are likely to develop a cancer. For this reason, medical scientists use different types of software to identify cancer cell or to decide weather a tumor is malignant or not. Using a software, they could perform various kinds of analysis and processing on imageries obtained from scans such as MRI or CT Scan {al2012lung}. An example of software that is used for cancer imaging research is DMRI. Such software is extensively used by many researchers, more than 75,000 downloads every year {norton2017slicerdmri}. Therefore, it is clear that software plays a critical role in medicine, to diagnose diseases and ultimately to save life.

Software plays an important role in power system planning and operation as well. One of the major activities in power system operation is contingency analysis. During contingency analysis, engineers determine violations of power grid operation conditions, such as overloading, which might occur when outage of a transmission line or a power generation unit happens. Contingency analysis helps to understand power system behavior after outages and gives an opportunity to take preventative actions {mishra2012contingency}. Power grids are extremely complex and such kind of analysis tasks are unimaginable with out a use of software. An example of software that is used to perform contingency analysis in the power system operation is Power World software {powerworld.com}.

Though it is not possible to mention the role and use of software across all areas of science and research, the above examples serve to be a good sample to see how ubiquitous the impact of software is almost in all research areas of science.

## The role of software in research breakthroughs

The impact of software is more pronounced and easy to observe when scientists achieve ground breaking results and the use of software enabled scientists to produce better scientific discoveries and achieve research breakthroughs {goble2014better}.

One good example of research breakthrough made possible, because of use of software in a scientific investigation, is creation of the very first visual representation of a black hole using an open source software NumFOCUS {event2019first}. To observe a black hole that is 55 million light years away, it would have required to build a huge telescope of size of planet earth. But instead of building one giant telescope, which is not possible any way, hundreds of scientists spent decades of years creating a global network of telescopes, known as Event Horizon Telescope (EHT) {enwiki:1052167868}, synchronized precisely using atomic clocks.

The EHT gathered a huge amount of data for years. However there was a lot of noise in the collected data because the EHT was a network non-similar telescopes. In addition, the radio signals were coming through attenuated due to atmospheric effects like water vapor, clouds, turbulence … etc. { <https://numfocus.org/case-studies/first-photograph-black-hole> }.

Therefore the scientists had to use various algorithms and data analysis pipelines. The resulting image from various data processing was compared to ensure the integrity of the result. This huge scientific breakthrough in a space research, can be attributed to the use of powerful data processing software.

## Summary

In this chapter, it has been explained how important and pervasive software in a scientific research is and the impact overall. The next chapter focuses to identify main categories of software usage purposes from the literature and software ontologies.

# Software usage purpose

## Introduction

In scientific investigations broad range of software is being employed for various purposes. In terms of size, software ranges from simple script to extremely complex one with millions of lines of code. In terms task, a software can be used for execution of rudimentary tasks to computation of extremely complex ones. Typical examples of purpose of software use for scientific investigation are simulation, modelling, data analysis, etc. {goble2014better}.

To be able to automatically identify, from context, for what purpose a software is used in a scientific text, a classifier algorithm has to be trained on a manually annotated dataset that indicate software usage purpose. The SoMeSci data set already has annotations about type of software, type of software mentions, etc. and only require extension with software purpose annotation so that it can be used for training a software usage purpose classifier. However, a comprehensive list of potential software usage purposes has to be identified before hand. To enumerate possible software purposes of usage, three things have been done in this thesis. These are:

1. Analysis of literatures
2. Analysis of software ontologies
3. Analysis of Sci-Crunch repository

After identifying a list of potential software usage purposes, the list has been consolidated further to narrow down the list to a more comprehensive list of software usage purposes for convenience during annotation of data set.

This section elaborates the analysis procedure of a list of resources mentioned above to identify possible software usage purposes.

## Analysis of literatures

In a research, scientists follow scientific method to discover knowledge. Typically, scientists begin with a question and attempt to answer questions through a research and propose hypothetical answers for their questions. Then, they test the proposed hypothesis by conducting various experiments. Although all scientists do not follow the exact same procedure, the over all idea remains the same {enwiki:1061107378- Scientific method}. This is where a software use comes into play, aid scientists during their experiment. Therefore, the analysis of literatures when looking for software usage purpose is aimed at answering, from a given context, “*for what purpose scientists are using a software ?”* in their experiments. Accordingly, some key words that reflect potential software usage purposes have been identified from the literature and listed on the following table:

|  |  |
| --- | --- |
| * Comparison of experimental groups * Quantification * Measurements * Analysis * Mapping * Correction of mapping * Generate scaffolds * Generate trees * Search sequences * Map * Predict gene structure * Align gene * Filter * Evaluate * Select * Optimise * Classify | * Statistical analysis * Data analysis * Densitometric analysis * Voxel-based Analysis * Cross-sectional ROI analysis * Gene analysis * Gene assembling * Construct contigs * Fill gaps * Generate assembly * Calculate or determine a value * Draw heat map * Validate * Annotation * Fit or train a model * Sketch * Identify |

The list of key words in the above table is used to delineate possible software usage purposes, however, it is intractable to enumerate all possible software purposes by manually reading through unlimited number of publications. To augment results obtained from the analysis of literature, various software ontologies and repositories like, Sci-Crunch, have been analyzed as presented in the following section.

## Analysis of software ontologies

Ontologies are controlled vocabularies that provide formal naming and definition of properties and relation between concepts, entities, data etc. Ontologies are specialized to a specific subject matter and every academic discipline creates ontologies to organize data into useful knowledge {enwiki:1060388948}.

Effective knowledge representation begins with analysis of ontologies with in the domain of interest {chandrasekaran1999ontologies}. Accordingly, analysis of software ontologies have been done to find out possible software usage purposes. The software ontologies, that has been analyzed on this project are: WikiData, SWO (the software ontology), and OntoSoft.

### WikiData

Wikidata is a multilingual knowledge graph that is curated collaboratively by a Wikimedia community and serves as a freely available common source of structured data for everyone {enwiki:1060114687, enwiki:1060408581}.

Wikidata was created by Wikimedia foundation mainly to store meta data that can be used for other Wikimedia projects such as Wikipedia. Interestingly, wikidata is allowed to contain inconsistent and contradicting facts in order to embrace the diversity of knowledge about a given entity {vrandevcic2012wikidata}.

Although wikidata has a tremendous amount of data in it, there was no information that would indicate software usage purposes, rather information about software categories was found. Therefore, an indirect approach has been taken to list down possible software purposes from software categories by assuming each software category has essentially a software purpose associated to it.

Wikidata comes with a bunch of tools like, SPARQL end point, query builder, data visualization tools, etc. Thus a SPARQL end point has been utilized to query a list software and their potential categories in a format that supports network analysis, with edge and node. {Take a look at the SPARQL query used on the Appendix}. As a result, over 400 software categories have been found from the Query.

To find out potential relation between these categories and to select more general software categories, a network analysis has been done using Gephi software (version 0.9.2) (RRID:SCR\_004293){<http://gephi.org/>}. Using Gephi, clustering of related software categories and filtering has been made to identify a more generalized software categories. The procedure for network analysis has been described as follows:

1. First query result from the SPARQL terminal of wikidata has been downloaded in a csv file format, with a data structure that supports node and edge.
2. Then, the csv file has been opened with Gephi software as “undirected graph”. This renders a network graph with overlapping nodes and edges.
3. To unravel the overlapping nodes for visibility, the lay-out of the graph is then changed to “Fruchterman Reingold”.
4. To find out possible clusters from the network, from the list of statistical tools, “Modularity” has been run. Then nodes and edges has been partitioned using “Modularity class”.
5. Then to adjust size of nodes based on importance, node size ranking has been done with a “Degree” parameter with {minimum, maximum} size of {20, 80} respectively.
6. Then to select the most prominent nodes, among filter tool “Degree range” filter has been used. The Degree range filter estimated prominence of the nodes between values of {1, 60} where the maximum value indicates the most prominent node which corresponds to a more general software category.

Text

Description automatically generated

Text

Description automatically generated

Degree {3, 60}

Degree {1, 60}

Timeline, map

Description automatically generated

Diagram, map

Description automatically generated

Degree {7, 60}

Degree {5, 60}

According to the network analysis, major types of software categories (prominent nodes in the network graph) are:

* Application software
* Utility software
* Computer security software
* System software
* Client
* Programming tool
* Software Library
* Software framework
* Editor
* Science software.
* Graphics software
* Computer aided design software
* Mathematical software
* Communication software

The above software categories are related to each other as well. According to a manual analysis of wikidata, mathematical software, for instance, is subclass of science software and science software is subclass of application software. By further analyzing the relation between the above software categories, overall three main types of software categories have been identified as follows:

1. Application software
2. System software
3. Software Component

A simplified version of relation between software categoriesis depicted on the grapgh below.

Diagram

Description automatically generated

#### Identifying software purpose

The main aim of software category analysis of wikidata was to find possible software usage purposes from each software category. It is simple to define a software purpose when the software is dedicated to carry out only a specific task.

One of the three main software categories is application software. According to Wikipedia, an application software is a computer program that is designed to carry out a specific task other than operation of a computer and typically made for end-users {enwiki:1060918552}. Most of research software can be considered as an application software, since they are used for a specific purpose.

However it is also worth mentioning that, there are two types of application software: horizontal (market) application software and vertical (market) application software. A horizontal (market) software is a kind of application software that is more generic, used in wide range of industries, and lack very specific purpose { enwiki:1034388659}. Examples of such types of software are word processors, spreadsheets, calendar applications, etc. On the other hand there are Vertical (market) application software whose purpose is to address needs of a specific niche in a business, research, or even a specific department within an organization {enwiki:879502666}.

Since purpose of software is of interest for this project, emphasis has been given only to application software only which imply a specific purpose of use in research papers. Accordingly, sub-categories of application software with their respective purpose from Wikipedia and internet resources have been gathered and summarized on the following table.

|  |  |  |
| --- | --- | --- |
| Types of Application software  (sample) | Software purpose | Examples |
| Remote sensing software, | * Data collection * information gathering | * Google earth, * OpenEV * ENVI |
| Econometrics software | * Data Analysis | * Stata * R * SATA * SPSS |
| Network simulator | * Simulation | * OPNET * NetSim * GloMoSim |
| IDE , text editors | * Programming * text editing | * Visual Studio, NetBeans, * Atom, Sublime, Vim … etc. |
| Genealogy software | * Record data, * Organize & publish data | * Family Tree builder * Legacy |
| computer-aided design software | * Modelling * Analysis & optimization | * AC3D, SolidWorks * AutoCAD, CATIA, … etc. |
| * Science software, Bioinformatics software, mathematical software, chemistry software,   astronomy software | * Simulation * Modelling * Data Analysis * Visualization * Calculation |  |
| database application | * Retrive, Insert, modify, delate data |  |
| graphics software , animation software | * 3D modelling, * visualization | * 3D computer graphics software, |

In summary, from the analysis of software categories of wikidata ontology, the following list of software usage purposes have been identified:

* Data recording or collection
* Data Analysis
* Visualization
* Simulation
* Modelling
* Programming.

### The software ontology (SWO)

The software ontology (SWO), particularly describes software used, for preparation and maintenance of data, within fields of computational biology and bioinformatics. The SWO was primarily developed to improve reproducibility by providing detailed description about software used for biomedical investigations {malone2014software}.

SWO was found on ontology search (OLS) website and was examined for possible software purposes. Unlike wikidata, a list of possible software purpose were found directly in “browse terms” section of the SWO website. To navigate to the list of key words that suggest potential software purpose one can follow the following steps: “Browse terms”> “entity“>”occurrent”> “planned” >”planned process”. The software usage purpose in the SWO has been presented in to two main groups as “data transformation” and “data visualization”. Under data transformation, 40 sub-types of potential software purposes are listed.

Graphical user interface, website

Description automatically generated

After manual analysis and grouping of purpose of use of software, more general classes of software usage purposes has been summarized on the table below:

|  |  |
| --- | --- |
| * Data transformation * Annotation * Text editing * Modelling * Curve fitting * Simulation * Query and retrieval | * Calculation * Analysis * Data visualization * File rendering * Matrix manipulation * Data mining task * Clustering task |

### OntoSoft

Onosoft is a software registry framework that stores important metadata about software to foster reuse and sharing of software among scientific community. The ontology provides descriptions about a software that would help scientists to identify, understand, execute, and do research with a software. Moreover, it helps scientists get information about update and support for the software. These descriptions are visualized in a 6 dimensional pie-chart, with each slice indicating the completeness of the description. Particularly, Ontosoft focuses on the geoscience because software resources are not being shared adequately in that field {gil2015ontosoft}.

Graphical user interface

Description automatically generated

The type of information provided in each dimension of description entries are summarized in the table below:

|  |  |
| --- | --- |
| Dimension | Description |
| Identify | * Name of software, abbreviation of the software, etc. |
| Understand | * Creator of the software, publisher of the software, * *domain specific key words* |
| Execute | * URL for downloading the software, license, system requirements …etc. |
| Do Research | * Input / output file formats, preferred citation information, …etc. |
| Get support | * Contact details, possible support included, etc. |
| Update | * Version, developer community, software development process , maintenance, etc. |

From the set of information provided among the 6 dimensions of the Ontosoft, particularly the “understand” dimension has nearly 400 domain specific key words that would potentially indicate software usage purposes. Therefore, those domain specific key words has been retrieved, analyzed and condensed into a more general software purposes.

Sample list of domain specific key-words that would potentially indicate a software usage purpose is listed on the following table.

|  |  |
| --- | --- |
| Domain Key-words | |
| * Data manipulation * Data Mining * Image processing * Machine learning * Simulation- optimization * Network analysis | * Numerical model * Numerical simulation * Thermal model * Integrated modeling * Interactive visualization * Wind wave estimation |

## Analysis of Sci-Crunch repository

The other resource analyzed in addition to software ontologies is to list down software usage purposes is Sci-crunch repository. Sci-crunch is a data portal that searches through hundreds of community databases, aggregates information resources to create a large collection of data and tools available for access at a single spot {grethe2016scicrunch}.

To identify possible software usage purposes, the Sci-crunch repository has been analyzed as follows. On the registry section of the sci-crunch home page, there is a pie chart indicating different types of resources. A software resource, with 7,155 different types of software resources has been selected from the pie chart. From there, top 200 types of software resources have been identified using the site’s built in word-cloud generator.

Text

Description automatically generated

After a manual analysis of the 200 of software types, generated from the word cloud, important software types that indicate possible software usage purpose has been identified. Sample of software types and their corresponding usage purpose is shown on the table below:

|  |  |
| --- | --- |
| Type of software | Purpose |
| * Data acquisition software * Image acquisition software | * Data collection * Data recording |
| * Data Analysis software * Image analysis software * Sequence Analysis software * Network analysis software * text-mining software * signal processing software | * Data Analysis |
| * Data Visualization software * 3D visualization software | * Data visualization |
| * Simulation software | * Simulation |
| * Alignment software , Image reconstruction software | * Data pre-processing or post processing |
| * Rendering software | * Modelling and graphics |
| * Code testing framework | * Programming |

## Types of software usage purposes

Based on a through analysis of scientific literatures in **SoMeSci** dataset, software ontologies and the sci-crunch repository, overall 8 main types of software usage purpose have been identified. These are:

1. Data Collection
2. Data pre-processing
3. Data Analysis
4. Data visualization
5. Simulation
6. Stimulation
7. Modelling
8. Programing

The overview of work flow process followed to identify these software usage purpose is summarized in the picture shown below.

*Diagram

Description automatically generated*

To establish a clear boundary and avoid ambiguity during the annotation process of software usage statements, in SoMeSci data set, each software usage purpose has been clearly defined based on literature in the next section as follows.

### Data collection

According to Wikipedia, data collection is a process of collecting, recording or measuring information on targeted variables which enables answering of questions. Regardless of the type of data, quantitative or qualitative, data collection is one of the most important steps in a scientific investigation {enwiki:1049936190}.

Scientists collect data for their research using various data collection software tools and gadgets. In one research, for instance, scientists used an Actigraph Reader Interface Unit (RIU-41A) with its software to measure the level of activity of more than 5000 children of age 12 to characterize the relation between physical activity and obesity {ness2007objectively, enwiki:1046731490}.

### Data pre-processing

Data collection processes produce inconsistent data and analysis of such noisy data might yield misleading results because of the “*garbage in, garbage out*” problem {enwiki:1059558941}. To avoid this problem, scientists usually carry out data pre-processing using a software. Data pre-processing generally refers to the addition, deletion, or transformation of raw data into a clean and tidy form to improve performance and reliability of analysis results, especially in data mining applications {kuhn2013data,rinnan2009data}.

Often times data pre-processing involves several steps such as data cleaning, integration, transformation, reduction, etc. {malley2016data}. Data cleaning, for instance, involves dropping of data, replacing, or imputation of missing values in order to improve performance of algorithms and reliability of analysis results, especially in data mining applications {enwiki:1051181443, enwiki:1056727993}.

In a scientific investigation, scientists usually carry out data pre-processing using a custom script or using an existing application software or programming library.

*From here add examples from* ***SoMeSci*** *data*

### Data Analysis

Data analysis refers to processing, transforming, modelling, etc. of data with *a goal of discovering a new insight* that would support conclusions or decision making. Data analysis involves diverse techniques with different names in various domains. {enwiki:1061024140}. In their research, scientists employ various software to carry out various tasks of data analysis such as curve fitting, spectral smoothing using a software {proctor1982data}.

### Data visualization

Data visualization refers to techniques that are used to communicate data or information effectively in the form of visual objects such as points, lines, bars, etc. in a graphic representation {enwiki:1059912747}.

### Simulation

Computer simulations mimic operation of real-world process or system using models that represent key-behaviors of the system. By varying variables of the simulation, predictions about behavior of systems can be made. Simulations have a wide range of application in scientific modelling of natural systems in physics, chemistry and biology {enwiki:1061669086}. Simulations are run to improve understanding of a problem (segal2008developing).

### Stimulation

Stimulation is the act of evoking the development of involuntary activity or response. Living organisms have sensory receptors that generate impulses that travel through nerve to the brain upon a reception of excitation by means of various agents, energy, collectively known as stimuli. Examples of sensory receptors in the human body are photoreceptors in the retina, touch receptors on the skin, chemical receptors in mouth, etc. {enwiki:976395276}.

In the scientific investigations, scientists use various mechanisms to provide a stimulation to their research object. One of the ways to provide stimulation is using a software. In neurological research, for example, scientists use various brain stimulation techniques and software to study neurological disorders. Deep Brain Stimulation (DBS), for instance, is one of brain stimulation techniques used to treat diseases like Parkinson’s, essential tremor, dystonia etc. {schermer2011ethical}.

### Modelling

Modelling refers to scientific activities that aim to facilitate understanding of a particular feature or phenomena in the world. It is a process of identifying and selecting relevant aspects of a situation or phenomenon under consideration. Different types of models with more specific aim exist. For instance, conceptual modelling provide better understanding, mathematical models help to quantify, computational models are used for simulation, etc. {enwiki:1051627717}.

Modelling is a broad term that refers to a wide range of activities. It might refer to 3D modeling and graphical representation of a real world physical objects like vehicles, buildings, …etc. using Computer Aided Design (CAD) software. For instance, some scientists use graphical modelling software, for instance for digitally documenting historical sites such as castles {el2007detailed}. On the other hand modelling can also refer to mathematical representation of a non physical abstract entity. In one research paper, for instance, the researchers were trying to model the occurrence of letters and word’s initials mathematically {pande2010mathematical}.

Regardless of the wide meaning and techniques of modelling, inherently all models serve to represent an object or a system to facilitate the representation, or understanding of particular feature or phenomena {enwiki:1058944086, enwiki:1051627717 }.

### Programing

Programming refers to the process of designing and building executable computer programs that performs a specific task. Computer programs are written in a human readable format mainly to automate execution of complex tasks and for solving problems {enwiki:1062649903}.

## Summary of scope definition for software purposes

|  |  |
| --- | --- |
| Software Usage Purpose | Scope |
| Data Collection | * Surveying * Data acquisition * Text extraction * Measurement * Data recording * Constructing an artificial data set * Importing a file or data of specific format into a software, etc. |
| Data pre-processing | * Data cleaning * Data encoding * Text editing * Error correction * Data normalization, calibration, data type conversion * Missing data handling, removing duplicates * Data transformation, data format conversion * Data reduction * Tabulating, merging data * File formatting * Aligning gene |
| Data Analysis | * Sequence analysis * Data manipulation * Testing hypothesis * Data mining , clustering * Prediction * Quantification * Calculation, computation * Comparing, testing, searching, * Assessing / evaluating * Densitometric Analysis * Image analysis /processing * Mathematical analysis * Network Analysis * Numerical Analysis * Regression Analysis |
| Data Visualization | * Creating figures * Plotting * Graph generation * Figure generation |
| Simulation | * Flight simulation * Event simulation * Flood dynamics simulation * Numerical simulation * Simulation of vehicle schedule |
| Stimulation | * Stimulate behavior |
| Modelling | * Scientific modelling * Mathematical modelling * Machine learning / Model fitting * Predicting a behavior * Estimating * Inference |
| Programming | * Implementation * Programming |

# Data set

## Introduction

Training and evaluation of automatic information extraction approaches requires availability of reliable ground truth data of sufficient size. Following a growth of interest for extraction of information about software tools from scientific publications labeled data sets with limited scope such as BioNerDs, SoftCite, SoSciSoSci have came into existence. More recently, SoMeSci data set, a more comprehensive corpus that covers a wide range of information about software tools has also been introduced {schindler2021somesci}.

This section describes the data set used in this project – SoMeSci, the extension process with software usage purpose annotations, issues observed during annotation, pre-processing of the data-set, analysis results of the data and transformation to a suitable format for training purpose.

## SoMeSci data set

SoMeSci data set contains high quality, hand annotated articles collated from PubMed Central (PMC). The articles and annotations included in the data set are summarized below.

### SoMeSci Articles

The corpus is composed of four group of files, namely *PLoS methods*, *PLoS sentences*, *PubMed full text* and *Creation sentences*. Facts about the articles in the SoMeSci corpus is summarized in the table below:

|  |  |
| --- | --- |
| SoMeSci parts | Description |
| *PLoS methods* | * 480 files * Contains only methods sections extracted from PLoS journal |
| *PubMed full text* | * 100 files * Randomly selected 100 full-articles from PMC Open Access |
| *PLoS sentences* | * 677 files * Contains sentences extracted from 677 PLoS articles * sentences contain software names. |
| *Creation sentences* | * 110 files * Out of 110 files, 50 are extracted from PMC OA * Out of 110 files, 60 are extracted from PLoS * Sentences contain statements that indicate creation of software. |
| *Total* | * 1367 files |

### SoMeSci Annotations

SoMeSci corpus has three main types of annotations that correspond to a type of information related with software tools. These annotations indicate the *type of software*, *type of mention* and *additional information* about the software as summarized on the table below:

|  |  |
| --- | --- |
| software information | Description |
| Type of software  (4 - types) | * Application * Plugin, * Operating System and * programming environment |
| Type of mention  (4 - types) | * describes the software’s appearance in the publications. * *Mention* – indicates software was just mentioned in the article * *Usage*- indicates software was used for some reason * *Creation* – indicates novel software is produced or introduced * *Deposition* – indicates deposition of new software in a repository. |
| Additional information  (9 -types) | * *Developer* * *Version* * *URL* * *Citation* * *Extension* * *Release* * *License* * *Abbreviation* * *Alternative name* |

## Annotation tool

The data set has been annotated using BRAT rapid annotation tool, v.1.3 RRID:SCR\_008769, in a Linux 20.4 environment. The annotation tool has been run in a local machine as a CGI application using a browser.

Graphical user interface, text, application

Description automatically generated

### Annotation of SoMeSci with software purpose labels

SoMeSci corpus has been extended with annotations of eight classes of purpose of software usage labels identified in the earlier section. Since using software for a particular purpose only refers to the usage of a software, only usage labels has been further labelled with software purpose. The figure below shows SoMeSci data set before and after software purpose annotations.



A picture containing text

Description automatically generated

### Challenges during Annotation

Annotations has been carried out in a such way by deciding on each context which software purpose annotation is more important or based on the general goal of the software usage. For example, FlexArray software on the figure below, has been annotated with software purpose analysis even though the same software was used for visualization purpose as well. This is because on this context analysis is more important than visualization and essentially visualization could also be interpreted as one kind of analysis. In addition, specific definition of each of software usage purposes has been also taken into account.



However, annotation of software usage statements was not often straightforward. This is because, in some instances as shown in the figure below, purpose of software usage might not be clear from the context.

{PICTURE}

More over, in some cases possibility of multiple candidate labels for a given software usage label was also observed. For example in an example below

{PICTURE}

The other challenge of annotation was difficulty arising from limited domain knowledge.

## Data Pre-processing

Pre-processing of the data set has been carried out to ensure the integrity of our data set before using it in the classifier. The data pre-processing tasks handled annotation errors, merging software-purpose labels with software-usage labels, transforming and splitting of data set.

### Handling annotation errors and missing annotations

As described in the above table, the four types of software mentions in the SoMeSci are *mention, usage, creation* and *deposition*. The main goal of annotating the data set was to assign corresponding *purpose* of software usage label to each instance of software *usage* but not for *mention*, *creation* and *deposition*. However, due to an error there were some instances of software *mention* that has been annotated with software purpose. In addition to this, there were also some instances of *usage,* that has not been annotated and intentionally skipped because of the purpose of software usage did not seem to be clear.

Therefore, all instances of wrong or missing annotations have been identified automatically identify to ensure the integrity of our data set.

### Merging annotations

After handing all annotation errors and missing labels, annotations of software usage have been merged with annotations of software purpose mainly for two reasons. The first is to fix annotation error message that is displayed on the BRAT tool. The error message is displayed because more than one annotation per a token is not supported by the annotation tool.

The other reason for merging annotations is to take advantage of legacy code, ariclenizer, which will transform data format from BRAT’s stand-off format into IOB format which is desirable for training purpose.





### Transformation to IOB format

After merging software usage and purpose labels, transformation of data into IOB format{enwiki:1041803321} has been carried out using articlenizer (link to articlenizer). Picture below shows the data format before and after transformation.





### Data Splitting

After the data has been transformed into the IOB format, it has been further split into training, development and test set in 60:20:20 ratio.

## Analysis of Annotated Data

Analysis of cleaned SoMeSci data set has been carried out to find a deeper insight about the training data.

### Co-reference resolution of software entities

The base line for the analysis of the data set was to carry out disambiguation of software names. This was particularly important because there is large degree of variation in software names. Using list of software name with corresponding [URL](https://github.com/dave-s477/SoMeSci/blob/master/Linking/artifacts.json), software mention instances have been disambiguated from each other and all software name variations that refer to the same entity have been given the same name. Figure below shows name variations for MATLAB software, in which all instances resolve to the same URL i.e. entities referring to the same software. All variations of names has been replaced by the first “Matlab” in this case.

Text

Description automatically generated

### Analysis results

According to the analysis results, the top 3 software by number of software name mention count through out the list of articles in PubMed and PLoS data set are: PASW, GNU-R and STATA.

Chart

Description automatically generated

Data set analysis result from the perspective of purpose of software usage indicates that, the most common *purpose* of software usage are: *Analysis*, *Data pre-processing*, *Data collection* and *modelling* where as the least common are *simulation* and *stimulation*.

Chart, pie chart

Description automatically generated

Chart

Description automatically generated

The other insight form from the *software-type* perspective, is that the most commonly used type of software in the research articles in the data set is *Application* software.

Chart

Description automatically generated

When it comes to share of each purpose of software usage among the 4 types of software, the pattern once again clearly indictaes most of the time a software has been used for the purpose of *analysis* and *data collection* in all of the four software types.

A picture containing chart

Description automatically generated

Lastly, the most interesting insight that is important for the automatic classification task was determining: ” *for how many different purposes a given software have been used for* ?”. The analysis result reveals that from 657 unique software lists, a little over 3 out of 4 software have been used only for a single purpose. Over all almost 98% of software have been used for a purposes maximum of three. This indicates that most of the software have been used only for a specific purpose.

A picture containing shape

Description automatically generated

## Summary

This section has described the training data set, the annotation process and insights about the data. **One of the core results of the analysis result is the fact that most of the time, software has been used for a specific purpose[write this in the results]**. The next section presents models that could be suitable for classification of purpose of software usage statements using the data set described above.

# Classifier models

## Introduction

Software is a real world entity and its mentions in a scientific publications usually appear to be a sequence of tokens. Therefore, automatic classification of software usage purpose can be modelled as a sequence labeling task in which a class label, from a fixed list of class labels, is assigned to each token in a sequence.

Extraction of information about a software can be done following various approaches. In the past, rudimentary approaches such as searching for a term in paper, manual content analysis using human readers as well as rule based approaches have been employed (kruger2019literature). More recently a deep learning model have also been employed for extraction of information about software such as mention types, software type, etc. { schindler2022role}.

Sequence labelling is a type of pattern recognition problem, one branch of Natural Language processing (NLP). Examples of classical tasks of sequence labelling are part-of-speech (POS) tagging, named entity recognition (NER), and text chunking {akhundov2018sequence, he2020survey}.

Various types of models that implement sequence labeling can be broadly categorized as machine learning or deep learning based approaches {he2020survey}. Machine learning based models are Hidden Markov Models (HMM) {kupiec1992robust}, Maximum Entropy Markov Models (MEMM) {mccallum2000maximum}, and Conditional Random Fields (CRF) {lafferty2001conditional}. State-of-the-art sequence labeling model is based on Bi-LSTM-CRF a deep learning neural network architecture.

This section explores for models that are suitable for sequence labelling task of automatic classification of software usage purposes.

## Machine learning Models

### Hidden Markov models (HMMs)

One of machine learning models that are used for sequence labeling are Hidden Markov Models (HMMs). HMMs are based on Markov processes which describe a sequence of hidden finite states (Yi) in which a given state in a sequence depends only on the state prior it {enwiki:1071684499, enwiki:1068802172}.

As the model transitions through hidden states of Yi, it generates an observation Xi which corresponds to a token in a sentence {aggarwal2018machine }.

Chart

Description automatically generated with medium confidence

Figure 1: Hidden Markov model structure {aggarwal2018machine}

The Markov chain of hidden states generate observations based on its current stateusing a joint probability distribution p(x,s), hence HMMs are also referred to as generative models.

The challenge with Hidden Markov Models is that, it is difficult to define the joint probability because it requires enumeration of all possible observation sequences which makes inference intractable for most applications. In addition, observation sequences in most real-world applications have long-range dependencies and multiple features interacting together {bulla2006application, wallach2004conditional}.

### Maximum Entropy Markov Models (MEMMs)

Unlike hidden Markov models which generate sequences of tokens based on hidden states, maximum entropy models are discriminative models i.e., they model directly model the probability of each label Yi based on the current observation Xi and the prior hidden state Yi-1 {mccallum2000maximum}.

Chart

Description automatically generated

The biggest drawback with MEMMs and other discriminative directed graphical models based on Markov, tend to be biased in favor of states with fewer successor states {lafferty2001conditional}.

### Linear Conditional Random Fields (CRFs)

CRFs are similar with MEMMs in that both are probabilistic and discriminative models that can perform sequence labeling based on conditional probability p(Y|x) unlike joint probability of HMMs {wallach2004conditional}.

A picture containing chart

Description automatically generated

Figure 2: Linear CRF model {aggarwal2018machine}

CRFs differ from MEMMs in that they are undirected graphs, i.e., the inference of Yi depends on all the labels occurring before it as well as after it. This makes training of CRFs computationally expensive especially when a wider window of tokens is chosen to handle long range dependencies {aggarwal2018machine}. In addition to inability to capture long-range dependencies, CRFs have another problem, they capture context in a forward direction only {lample2016neural}.

## Deep Learning Models

Deep learning models yield a state-of-the-art performance for sequence labelling with out the need for manually crafting features because of their ability to automatically learn features from data {he2020survey}. In addition, deep learning models are advantageous because certain variants like LSTMs have the capacity to handle long-term dependencies {akhundov2018sequence}.

### Long Short-Term Memory (LSTM)

Recurrent Neural Networks (RNNs) are specific type of neural network architectures that take a sequence of inputs Xi and yield another sequence Yi as output. Plain RNNs fail to capture long-range dependencies however a there are other variant of RNNs, such as LSTM networks that are capable of handling long-term dependencies {akhundov2018sequence, lample2016neural}. This is because, unlike conventional feed forward neural networks, LSTMs have feedback mechanism that helps to capture entire sequence of tokens in a sentence enabling the network to remember tokens over arbitrary time intervals {enwiki:1073570927}.

Diagram

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<https://developer.nvidia.com/discover/lstm> img source { ma2016end }

A LSTM memory block has three multiplicative components, which determine what amount of information to remember as well as to retain to the next step {ma2016end}.

### Bi-Long Short-Term Memory (BLSTM)

Though LSTM captures the past sequence of tokens (on the left), it is not capable to capture future sequence of tokens. For this reason, two LSTM networks are combined to form Bi-LSTM where one captures context information in a forward direction while the other captures information in the reverse direction. This enables Bi-LSTMs to become aware of both past as well as future contexts {ma2016end}.

### Bi-LSTM-CRF

Bi-LSTM-CRF models are state-of-the-art, elegant solutions to sequence labelling tasks as they are capable of capturing context in both left and right directions due to their Bi-LSTM component.

Diagram, schematic

Description automatically generated

Due to its performance Bi-LSTM-CRF model has been employed for classifying software usage purpose from a sequence of tokens in a sentence. The classifier model implemented is a 4 layer network where each classifier layer is dedicated to classifying software, software-type, mention-type and software-purpose in respective order. Fully connected model is shown in the figure below.

Graphical user interface

Description automatically generated

### Word embeddings

To generate features for each word in a sentence, word embeddings like Sci-BERT and Bio-BERT have been used.

Sci-BERT is pretrained on multi-domain random collection, over 1.14M, of scientific publications and capable of generating contextualized embeddings for each token in a sequence. Most of the scientific papers used to train Sci-BERT are from biomedical domain (82%) and the rest from computer science domain {beltagy2019scibert}.

Bio-BERT is as well a contextualized word embedding trained on biomedical corpora. The scientific publications in the Bio-BERT corpora are made of abstract section of PubMed journal and full text articles from Pub Med Central (PMC).

# Model and Data Optimization

## Introduction

## Training scenarios and Hypothesis

## Optimization parameters

## Training Results

## summary

# Results and conclusion

## Summary of Results

## Conclusion

## Future work and limitations