

# Masters' Project Michaelmas Progress Report

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December 2015



## 1 Introduction

### 1.1 Modern Scientific Publishing

With the widespread adoption of the internet in the late 1990's and 2000's, there were fundamental sweeping changes in the academic publishing landscape. The information revolution allowed publisher's costs to fall dramatically, and there was a mood shift in the academic sphere away from subscription based models, towards giving open and free access to some or all of journal article contents.

Simultaneously, University Department websites began to post records of their recent publications for advertizing and informational purposes, usually with hyperlinks to where the article could be fully accessed.

Publishers still protect journal article content and metadata, in some cases, aggressively, in order to look after their intellectual property. The data they hold on article publishing is

immensively valuable, and as such, publishers are not willing to give access to their massive metadata holdings. There is a well known saying in Data Science from Tim O'Reilly, "The Guy with The Most Data Wins" [1]. As such, it is unlikely that academic publishing companies will release their data for analysis by the public.

## 1.2 Motivation

The publishing data, when collected and analysed using machine learning and big data techniques, can yield valuable insights into the direction of shifting academic focus, where world leading research is being carried out, and offers the possibility of procedural categorisation of research. The possibilities do not end there, and large datasets are almost infinitely mine-able for interesting insights. For an academic institution like the University of Cambridge, there are two main motivations for mining the data of the publishing landscape:

- Purely Academic insights such as examination of the landscape's features , finding structural information and concealed relationships, in order to better understand how scientific information is spread throughout the world
- Actionable insights, such as identifying where effective collaborations could be set up, prediction of where funding may be allocated, and identification of future areas of academic interests so that internal resources can be intelligently applied

## 1.3 Aims

There are two main aims for the project, broken down below.

- Data Collection - A scalable, legal and useful programmatic approach to scrape the online publishing landscape to collect as much useful data as possible.
- Data Analysis - Once the data has been collected, Machine learning and statistical techniques should be applied to try and find insights within the data.

The data analysis for such a large, rich dataset is a potentially never ending process. The strategy adopted is to focus on answering a smaller simpler research question first, building a structure to robustly test and answer that hypothesis and then to move on to new research questions. As such, the first research question will be to build a system that can analyse the similarity between scientific authors. This will enable us to find where some authors are publishing qualitatively similar work and to investigate the possibility of them collaborating. The framework upon which this research question is used immediately suggests new, similar questions that can be answered. As such, it will be a primary aim of the project to expose a useful framework for future probing to be facilitated.

## HTML and XPath

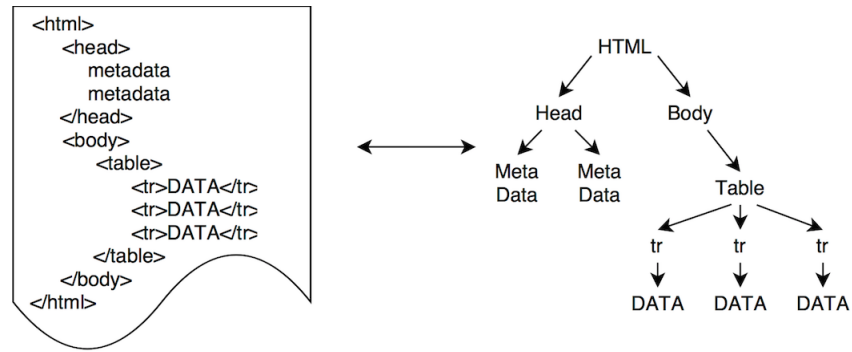


Figure 1: Tree representation of HTML code

From a technical point of view, the aims of the project are as follows:

- Provide documented, maintainable code
- Provide a system that is as automated as possible
- Provide a system that will automatically evolve and improve as time goes on
- Provide a system that will not entropically lose data or suffer data degradation
- Provide a system that produces interpretable, useful outputs

The focus is on ensuring that the result of the project is a system that will continue to be useful after the programmer has left. This will require decent documentation discipline, and systems in place to manage crashing.

## 2 First Steps

### 2.1 Generating XPath

The initial focus was on developing a strategy to scrape records off an unseen webpage. Webpages are written in a tree-like structure using a markup language called HTML, (HyperText Markup Language). A very basic webpage is shown in Figure 1

When a webpage is accessed, the html code is sent over the internet to the user, and the browser e.g. Firefox, interprets it and displays the webpage in a human readable format. When scraping a page for information, the html code itself is scraped. The programmer must write a program that accesses the useful parts of the webpage and stores the required information. In the above simplified example, it is shown that the html code represents

a tree structure, and the useful data is at the bottom of the 'body' branch. In order to store the DATA fields, the programmer must provide what is known as the XPath to that node in the tree. The XPath is just a direction to the data, and in the example above, the DATA fields are accessed via XPath:

`//HTML/Body/Table/Tr/*`

The XPath is a required part of any scraping strategy. The first problem with scraping potentially millions of webpages, is how the XPath (potentially very complicated, and certainly different for every single website) can be generated. The initial approach was to write a tree analysis suite that would give the XPath of the most 'probable' data entries. This worked by finding the most repeated substructure within the entire tree, and by using heuristics, parameters could be adjusted to automatically generate the XPath to the useful data with decent efficiency. The core of the algorithm is shown below:

1. Start at trunk of tree
2. Count the number of descendants of each child of the current node
3. (a) Check if all child nodes are all within a threshold of similarity to each other
  - (b) Check there are more than a required threshold number of child nodes
  - (c) Check the average similarity between child nodes is above a certain threshold
  - (d) Check that the proportion of child nodes that are considered 'similar' is above a certain threshold
4. If all of (a)-(d) are true, this node contains the required data and the XPath has been found. Otherwise, move down to the child node with the greatest number of descendants and return to step 2

The thresholds mentioned in steps 3.(a)-(d) are adjustable parameters set at reasonable values. This approach was successful for webpages with very large numbers of records on them, as the algorithm searches for the largest, most frequently repeating structural unit in the tree. If there are not vast numbers of records on the page, the method can fail. As such, it is not flexible enough a strategy, and whilst useful and still the quickest automated way to generate XPaths for webpages with many hundreds of records on them. A different strategy has been adopted, please see section 3.

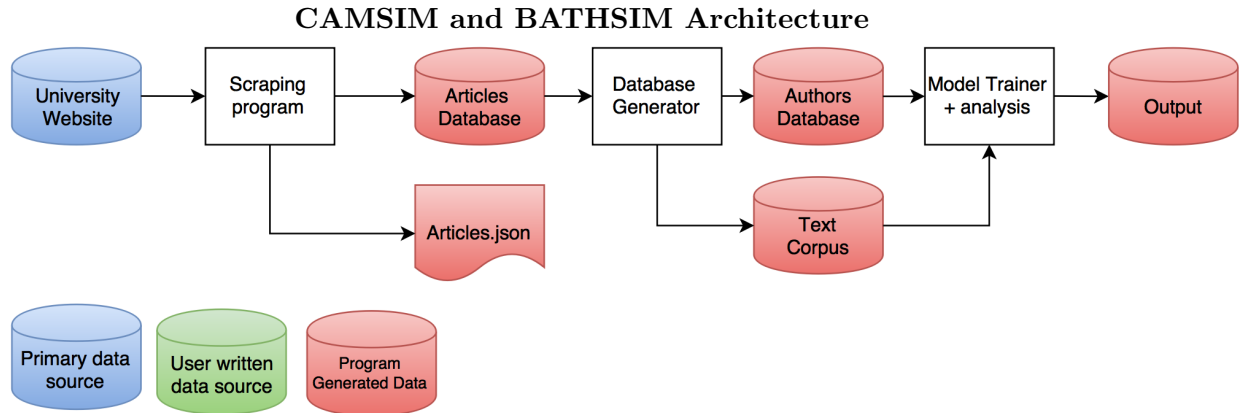


Figure 2: Flow Chart Diagram representing CAMSIM and BATHSIM structure

## 2.2 CAMSIM and BATHSIM Mini Projects

A significant part of the first few weeks of the project were dedicated to selecting and learning the appropriate technologies to achieve the goal. The CAMSIM and BATHSIM projects were small proof of concept projects to explore how the different technologies work together, and to prototype a system architecture. The technologies used are:

1. Python 2.7.10 programming language. A modern and flexible interpreted programming language widely adopted by the scientific community, python 2 has many useful libraries available, optimised for use.
2. MongoDB database - MongoDB is becoming one of the most popular databases for data intensive applications [CITATION NEEDED]. MongoDB is a schema-less noSQL database - it records objects as individual, unstructured elements rather than in tables. This is well suited to the task as complete data is not always available during large scraping operations. There are also well supported python drivers for MongoDB.
3. Anaconda Environment - Anaconda is a python distribution/virtual environment, allowing quick use of external python packages, and fast generation of distributions to deploy on new machines.
4. Scrapy Scraping suite - A well supported end to end scraping framework for python, allowing fast, scalable web scraping.
5. Gensim - A Natural Language Processing and Machine Learning suite for Python. Their libraries are C optimised and widely used and verified.

BATHSIM and CAMSIM projects use all of the above technologies with an architecture shown in Figure 2. The programatic flow is represented above. BATHSIM and CAMSIM

have the same structure, and the only difference is the source data for CAMSIM is provided by University of Chemistry Department at <http://www.ch.cam.ac.uk/publications> whereas BATHSIM’s source is the data provided by the Bath University Chemistry department, at <http://opus.bath.ac.uk/view/divisions/dept=5Fchem.html>. A custom written scraping program collects the data which is placed into a database and exported as a human readable .JSON text file. A second program then creates databases of individual authors and a corpus of all the titles and collected abstracts. As discussed in the section 4, this corpus is used to train a Word2Vec style model that generates a vector representation of an author’s published work. The dot product cosines between authors’ vectors are computed and outputted as a measure of their similarity.

### 3 Collection Strategy

The main problem encountered so far is how to scrape large numbers of websites for records without writing individual time consuming scraping scripts and finding XPath’s for every website visited, as was used in CAMSIM and BATHSIM. The possible solution is using ‘regular expressions’ pattern matching techniques on DOIs. DOIs are explained in detail in section 3.1. The proposed collection strategy, which is 90% complete, is then described in section 3.2.

#### 3.1 DOI

DOIs (document object identifiers) are identifier strings used access journal articles. DOIs can issued by a number of accredited issuing bodies, although the vast majority of scientific articles are issued by CrossRef, a not-for-profit body comprised from Publishers International Linking Association (PILA), a loose association of many academic publishers [2]. A DOI is usually included in a citation or record, and by pre-pending a DOI string with the url stub “<http://dx.doi.org/>”, DOI.org will redirect the request to the desired academic journal entry on the publishers website. All articles published by large established publishers will have a DOI registered against them.

DOIs have a somewhat loose structure, and the anatomy of a DOI is shown in figure 3.

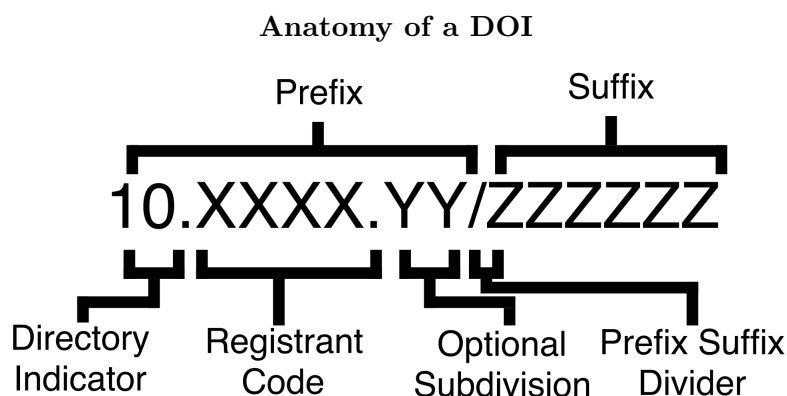


Figure 3: Doi structure. The structure consists of a numeric prefix (X and Y must be integers) and alphanumeric suffix (Z can be any UTF-8 encoded Character)

DOIs consist of 2 sections, the prefix and suffix. The Prefix is subdivided into a Directory indicator (always integer ‘10’) separated from a registrant code assigned by the issuing body. Registrant codes are numeric and can be of any length, however they are almost invariably 4 integers long. Registrant codes can have further subdivisions separated by full stops. The suffix is provided by the registrant themselves. It can have any form as long as it is encodable by UTF-8. This is somewhat ambiguous as there is no vigorous way to terminate a DOI, and on a webpage, the end of a DOI suffix must be interpreted from the context.

### 3.2 Cherry Data Collection Program

DOIs can be recognised programmatically from HTML source code through the use of regular expression pattern matching techniques. This suggests a way to collect article data without knowledge of the XPath. The strategy for creating a widespread scraping with well structured output data is summarised below.

1. Download page source of university website
2. Use pattern matcher to extract DOIs from the source HTML code
3. Verify scraped DOIs by using CROSSREF API service
4. Deposit valid DOIs in DOI Database
5. Use collected DOIs and DOI.org re-routing service to access publisher webpages for articles

6. Extract useful, freely available article data: Title, Authors, Date, Abstract, Affiliations

7. Store these full records in a database, for use in data analytics

This process allows widespread scraping as XPath's are only required for the publisher webpages, rather than the university websites. There are much fewer publisher website formats than potentially infinite formats for university websites, and a conversion rate of >90% has already been achieved on a sample dataset of DOIs to full records, from only ~20 publisher websites XPath sets. The algorithm above is to be implemented by the system architecture shown in figure 4

### Cherry Program Architecture

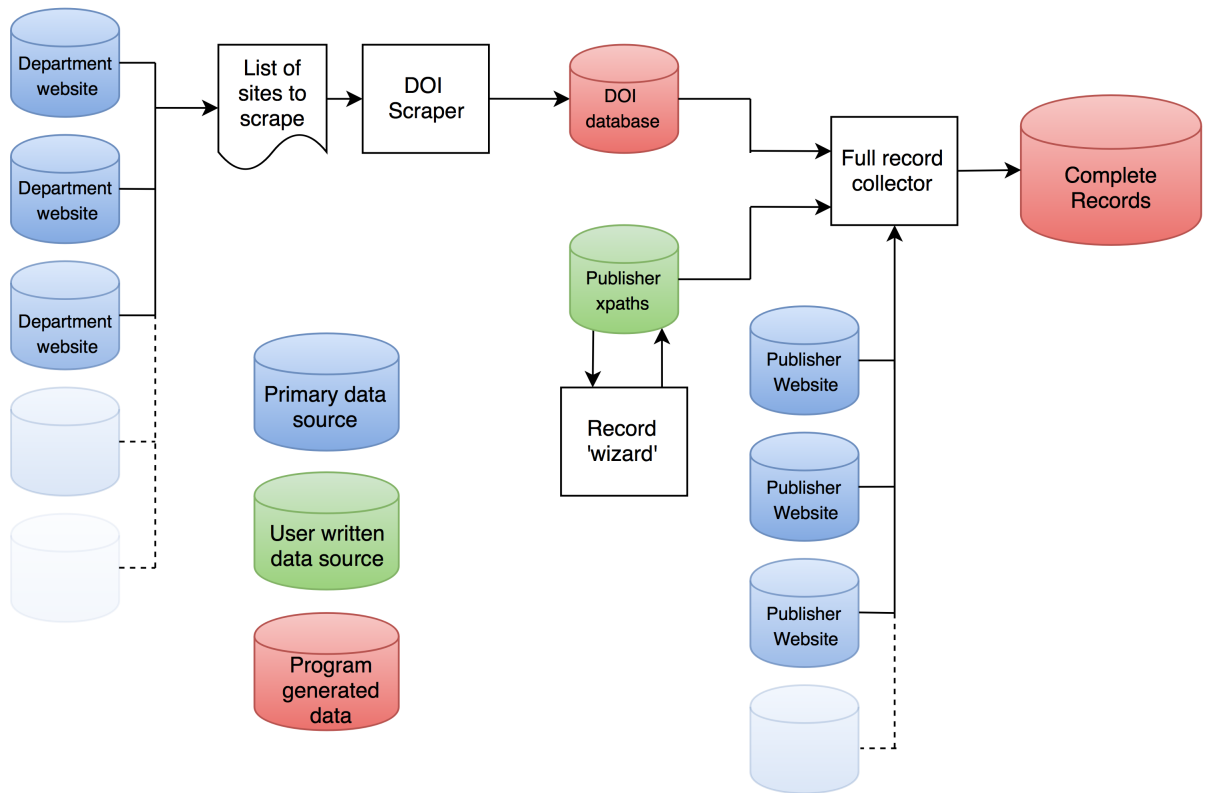


Figure 4: Flow Chart Diagram representing data collection strategy structure

The system has been named Cherry, as the process is somewhat like picking cherries off of an html tree, and then eating them. The naming convention of fruit runs through into the Analysis section. The Cherry data collection system is 90% complete at time of writing,



with the programs referred to in 4 as ‘DOI SCRAPER’ being complete and ‘Full Record Collector’ being put through thorough testing. The ‘Publisher XPaths’ database is an ongoing project, and can never be ‘Complete’. It is the only brittle part of the program and will necessarily need to be added to in order to incorporate more publishers and updated when publisher websites change. ‘Record Wizard’ is a proposed program to help write the XPaths and small normalisation processes required to collect full records for a given publisher website. As an auxiliary program not vital to the system to run, it is of lower priority and will be implemented when the system is up and running.

## 4 Analysis

### 4.1 Algorithm

The core aim is to be able to represent research interests quantitatively so that programmatic comparisons and analysis can be facilitated. The algorithm that will be used for this purpose is a recently published Natural Language Processing deep learning technique known as Word2Vec[4][5]. The Word2Vec algorithm is based off ‘continuous Skip-Gram’ and ‘Continuous Bag of Words’ architectures. These two learning algorithms are highly optimised, research level Natural language processing algorithms. The ‘Continuous Bag of Words’ (henceforth CBOW) attempts to predict the current word based on the word’s context (specifically the 2 words preceding and the 2 words following) during training and the ‘skip-gram’ model attempts to predict the surrounding words given the current word. They are, as such, mirror images of each other. The CBOW and Skipgram algorithms have different strengths but vigorous testing of which will be best of the task cannot be completed until a large set of training and testing data have been amassed. The CBOW appears to be better for syntactic relationships, and Skipgram better for semantic relationships[4]:

- Syntactic relationship: *good* is to *better* as *rough* is to ... (expected answer: ‘rougher’) [6]
- Semantic relationship: *clothing* is to *shirt* as *dish* is to ... (expected answer: some specific type of dish, e.g. ‘bowl’) [6]

The purpose of the task is to compare semantic chemical concepts, so it may prove that skipgram is a better fit for the purposes, however it will be an interesting question to compare outputs from either model.

The models themselves work in the following way. Sentences of words are assumed to contain words that are semantically and syntactically related. If two words appear in the same sentence, they can be assumed to be in some way ‘similar’. Word vectors are randomly initialised, and then iteratively optimised, so that weights of word-word connections in the

internal network are strengthened if that word pair appear often in sentences together. The procedure is somewhat similar to Neural Network techniques, with only an input and output layer (no non-linear hidden layers). The training complexity is greatly improved over Neural Network techniques.[4].

The end result of training the model on a corpus of data is that words are then representable as vectors within a language meaning space. These word vectors can be averaged together to aggregate sentences into concept vectors within the space.

## 4.2 Data processing

The database generated from the process described in section 3.2 contains much free text (the titles and abstracts of the articles). These are already composed of concept linked sentences and can easily be fed in as training data into the Word2Vec algorithms. The more data used in training, the better the model will be. This requires a database with a great many records[1][4].

A training corpus is prepared from the database of complete records in a processing pipeline described in figure 5

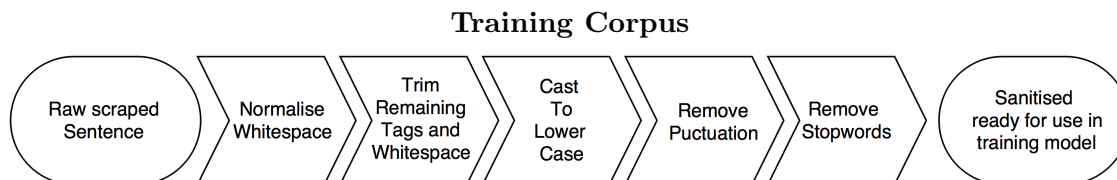


Figure 5: figure showing how data is sanitised and aggregated into the training corpus for training the Word2Vec model

#### 4.2.1 Author similarity pairs

#### 4.2.2 K-means clustering of research landscapes

#### 4.2.3 Tracking of Research interests with time resolution

### 4.3 Network visualisation

## 5 Next Steps

## References

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