

An Novel RNN Approach to Classification of Complex Textual Scientific Metadata

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Abstract

I introduce a new method for supervised classifying scientific metadata. This deep learning approach works with small and messy training data to provide high levels of accuracy. Using the method I analysis the introduction of new software tools to the statistics community.

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1 Introduction

Currently most analysis of scientific publications is limited to those fields available in the database used by the researchers. Efforts to extend the fields usually rely on unsupervised clustering (e.g. Boyack et al. (2005)). These methods are useful and have greatly increase our understanding of how science works as a social phenomena. But, if we want to find paper with properties not given in the standard databases the usual solution is hand coding, which is either time consuming or expensive (usually both).

Recent developments in deep learning (Karpathy and Fei-Fei, 2015) have been highly successful at labelling/classifying very complex inputs, usually text or images. These techniques rely on large training datasets which are not available for biometric tasks and thus very little work has been done with scientific metadata. By relaxing the purity requirements of the training data we show that sufficiently large training data can be generated and that it produces useful results.

The classification problem I am interested in is identifying *papers introducing new software packages, tools or interfaces*. This aspect of the literature has not been previously analysed like this due to data limitations. Thus this method allows me to with high confidences give broad statistics about software usage in statistics that have never been calculated before.

2 Literature Review

Computer's have been a formal part of scientific work since the 18th Century (Grier, 2013), but the modern day electromechanical machines developed by Turing (Turing, 1937) and many others (Abbate, 2012)(Abbate, 2000) are a much more recent innovation, of the last century (Bauer and Rosenberg, 1972). The introduction of these devices to communities around the world (both metaphorically and literally) has had major impacts on the culture (Lessig, 2007), technology(Abbate, 2000) and rate of development (Bauer and Rosenberg, 1972). Much work has been done to study these effects, but it has been primarily focused on either the macro cultural effects (Pfaffenberger, 1988) or the economic/business usage (Landauer, 1995).

By comparison the usage of computers by scientists has been overlooked by researchers (Lab, 2017). This oversight has many reasons, but one of the most significant is the lack of available data. The primary methods for large scale analysis of the culture or structure of scientific work involve bibliometric techniques (De Bellis, 2009) using large standard datasets(e.g. Boyack et al., 2005; Börner, 2010, 2015; Sugimoto et al., 2013; Shi et al., 2015; Evans and Foster, 2011; Skupin et al., 2013). These dataset are generally lacking information about the computa-

tional aspects of the work, e.g. the Clarivate Analytics Web of Science (WOS) does not have any such field (McLevey and McIlroy-Young, 2016) and as such research into this dimension is difficult. Recent developments in natural language processing (NLP) have shown that complex concepts can be extracted reliably from text for a wide variety of tasks (Evans and Aceves, 2016), with some very similar to that done here (Foster et al., 2015).

2.1 Information Extraction

To extract the information about software usage from the available data requires complex NLP techniques and the best methodologies change quickly(Evans and Aceves, 2016). As we are primarily concerned with the classification of meta-data for a record relating it to a new software tool or not, in theory there are a large number of available techniques, as this is a simple binary classification problem (James et al., 2013)(Jurafsky, 2000)(Murphy, 2012). We have considered most of the available techniques:

- Classified based on a simple regular grammar, e.g. regex
- Word collocation frequencies (Manning et al., 1999)
- Term frequency-inverse document frequency vectors with an SVM or other classifier (Collobert et al., 2011)
- Word2Vec vectors with an SVM or other classifier(Mikolov et al., 2013b)(Collobert et al., 2011)

The the current state of the art for natural language processing is the usage of deep neural networks for information extraction requiring more than simple word level similarities(Manning et al., 2014). As this is the state of the art there is no simple set of rules to follow, but there are some guidelines (Goodfellow et al., 2016). These have lead us to the use of a recurrent neural network (RNN) (Mikolov et al., 2010) for the classification, although the exact specifics have been determined with cross-validation techniques (James et al., 2013). The main features to consider are the type of regularization (Goodfellow et al., 2016), what representation of words to use (most likely Word2Vec (Mikolov et al., 2013b)), what non-textual data will be included as there are in the WOS data set over 60 possible fields for each record (McLevey and McIlroy-Young, 2016) and what values the hyperparameters take(Goodfellow et al., 2016). This tuning is highly specific to the data, framework (in this case PyTorch (PyTorch core team, 2017) with NVIDIA’s cuDNN (Chetlur et al., 2014)) and are described in further sections.

2.2 Data Analysis

Once the records with new software tools have been identified, we can use the existing theory of bibliometrics to look at the network structure. The literature standard approaches are to look at the structure of these nodes in the citation and authorship graphs (de Solla Price, 2002)(Larivière et al., 2006)(Borgatti et al., 2009). This can be a computationally intensive task but tools exists that make it more practical (McLevey and McIlroy-Young, 2017) so once the records have been labelled the analysis techniques are no longer novel.

The literature is silent on basic features of scientific software usage, and even when limited to only new releases there is no existing data. Thus simple measures such as per domain counts/frequencies and basic graph measurements such as the centrality will be new contributions.

The other main question of what causes tools to be successful, has not been answered for scientists. There has been some work in the business domain (Xin and Levina, 2008)(Hsu et al., 2009). The adoption of new tools by businesses is theorized to follow a sigmoid pattern, with successful new entrants having three stages of usage: First they are used by early adopters and have small market penetration. Then they reach a "take off point" and the large majority of users will adopter their tools. Finally there will be slow growth in adoption again as only the laggards are left as new users (Xin and Levina, 2008). This is based on adopters having a Gaussian distributed chance of adopting the tool and notably this diffusion model does not require that the software have any costs for the users and allows for network effects, thus this signature is considered in our modelling.

There also has been work done examined open source projects (Mockus et al., 2002) which agrees with the theory (Raymond, 1999) of open source that success is derived from openness and collaboration. This would predict that successful tools would come from highly connected groups who are working successfully with the community. This may show up as high connectedness in the co-authorship network correlating with success.

What leads to success has also be been studied in the context of ideas in the scientific literature (Acharya, 2004) (McLevey et al., 2016) or of individuals(Sinatra et al., 2016). In both cases the main measure of success is the cumulative count of citations, which we can also examine on a per paper and a per author basis. We can look for the predictors of success for a new software tool by examining its citations over time and us this as our measurement for the signature. Notably Sinatra et al. (2016) show a that success very unpredictable and can happen years after the paper is published. If the software records have patterns matching this model then the diffusion model may not be a good fit.

3 Data

The source of data used for this analysis is the Web of Science (WOS) database hosted by Knowledge Lab. It has metadata on almost all scientific publications from 1960 to 2015, with new records being more complete. Each publication can be linked to one or more other tables each which contain other metadata than the main table, the number of entries for each table I am concerned with are shown in Table 1 and the complete database schema in Figure 1. Access to the database is controlled by Knowledge Lab so they would need to be contacted to access it, once access rights are obtained the database is found at wos2.cvirc91pe37a.us-east-1.rds.amazonaws.com and the documentation at <http://docs.cloudkotta.org/dataguide/wos.html>.

The data for WOS were collected by Thompson Reuters until 2016, when it was given to Clarivate Analytics who now maintain it. The contemporary publications are collected from the publishers directly while older and more obscure publications are obtained from scanned copies digitalized with OCR, which is one of the factors that leads to newer publications having much higher quality data.

Table	Number of Entries
publications	57136685
abstracts	26093439
publishers	50668193
keywords	78155603
references	1085738245

Table 1: Web of Science database number of entries per table

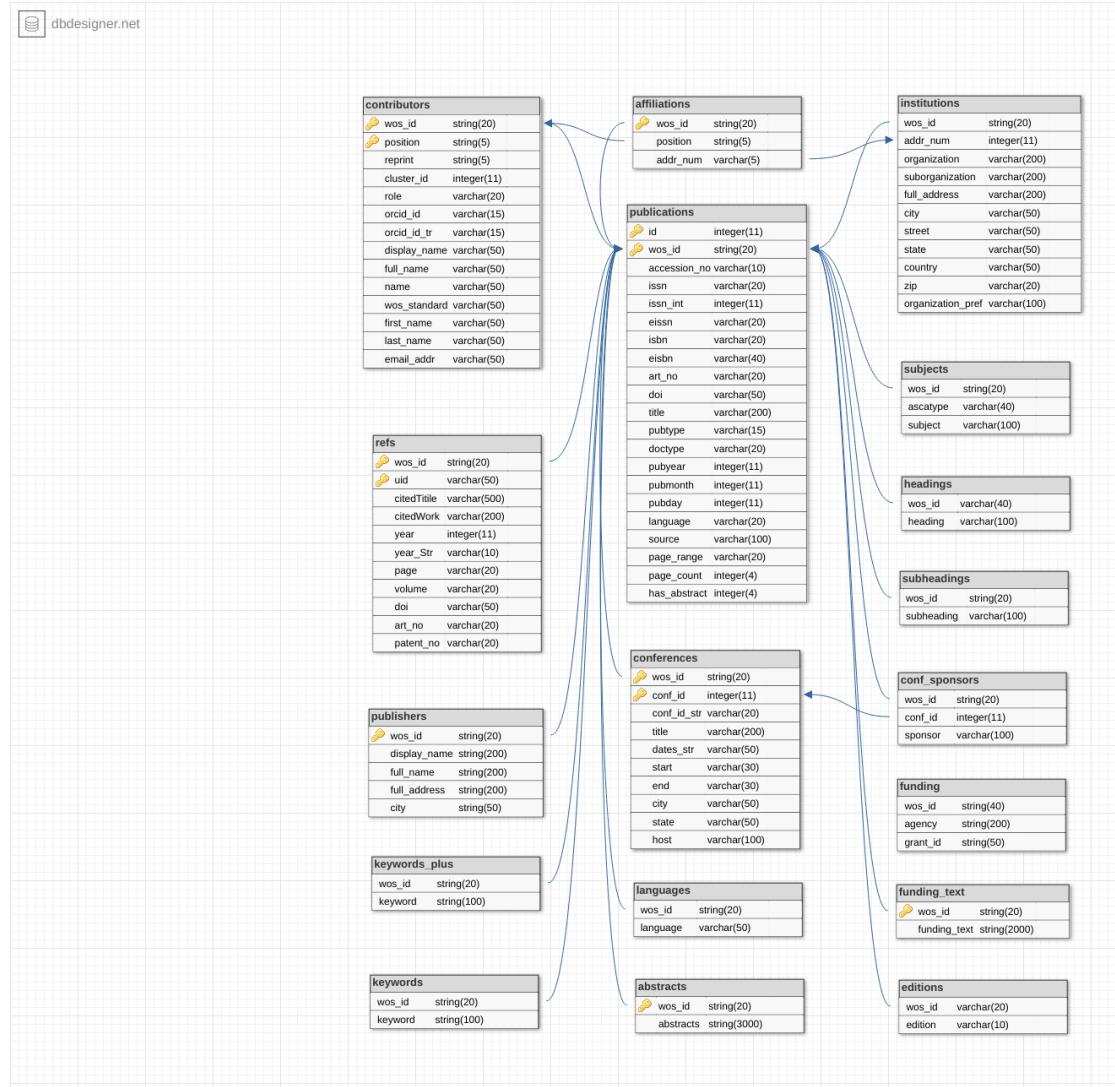


Figure 1: Knowledge Lab WOS database schema

For this analysis I limited my data to those journals from the top 123 statistics publications between 2005 and 2016, giving me a total of 78 971 articles (publications). From these I derived a training set of classified (training) and unclassified publications. To do this I found journals that almost entirely publish new scientific software, thus all articles from these can be classified as containing new software, i.e. as positive. There are also some that contain virtually none, all of their publications can then be classified as negative. The classified journals are given in Table 2, note they are all top statistics journals from the data set.

Journal	Classification	Total Citations	Impact Factor
R JOURNAL	Mostly Software	271	1.045
STATA JOURNAL	Mostly Software	2636	1.292
JOURNAL OF STATISTICAL SOFTWARE	Mostly Software	6868	2.379
ECONOMETRICA	Little Software	24957	4.053
TECHNOMETRICS	Little Software	6062	1.435
STATISTICAL METHODS IN MEDICAL RESEARCH	Little Software	2703	4.634
JOURNAL OF THE ROYAL STATISTICAL SOCIETY SERIES B-STATISTICAL METHODOLOGY	Little Software	2 360	1.702
BRITISH JOURNAL OF MATHEMATICAL & STATISTICAL PSYCHOLOGY	Little Software	1 278	3.698
ANNUAL REVIEW OF STATISTICS AND ITS APPLICATION	Little Software	74	3.045
ANNALS OF STATISTICS	Little Software	15 680	2.780
STOCHASTIC ENVIRONMENTAL RESEARCH AND RISK ASSESSMENT	Little Software	2 297	2.237

Table 2: Classified journals with 2015 citations and impact factors

When combined the I have a training set of 1251 positive and 4362 negative examples. This is not a large data set nor is it pure since some articles from the positive set are in fact negative, one example(Wickham et al., 2014) is shown Figure 2. As there is no pre-existing known set of clean papers I cannot give an exact count of the incorrectly identified papers, but as I will discuss later the model is capable of identifying them despite their presence in the training set. The paper used here is one of the one identified by the fully trained model as being not

software.

Field	Value
ID	WOS:000341806800001
Source	JOURNAL OF STATISTICAL SOFTWARE
Year of Publications	2014
Title	Tidy Data
Abstract	A huge amount of effort is spent cleaning data to get it ready for analysis, but there has been little research on how to make data cleaning as easy and effective as possible. This paper tackles a small, but important, component of data cleaning: data tidying. Tidy datasets are easy to manipulate, model and visualize, and have a specific structure: each variable is a column, each observation is a row, and each type of observational unit is a table. This framework makes it easy to tidy messy datasets because only a small set of tools are needed to deal with a wide range of un-tidy datasets. This structure also makes it easier to develop tidy tools for data analysis, tools that both input and output tidy datasets. The advantages of a consistent data structure and matching tools are demonstrated with a case study free from mundane data manipulation chores.
Citation	Wickham et al. (2014)

Figure 2: An example of a false positive in the training set

4 Methods

The classifier works as a series of operations on the two input strings (the title and abstract). The first step is tokenizing which is done with the Python NLTK package (Loper and Bird, 2002), this tokenizer is not perfect but it is deterministic and lossless which are both more important for this task. The tokens of interest are words and punctuation this string of tokens is then normalized to lower case and converted to Word2Vec (Mikolov et al., 2013a) word embedding vectors with gensim (Řehůřek and Sojka, 2010). The embeddings are from a model trained on the entire corpus of abstracts and titles using hierarchical softmax, with a window size of 5, as that is better with low frequency words(Mikolov et al., 2013a) than the alternative negative sampling (Mikolov et al., 2013b). NLTK’s sentence tokenizer was used along with its word tokenizer to generate the training sequences for the embedding, with titles treated as single sentences. The word embeddings primarily serve as a way of converting words into a vector space so the small sample size

is not an issue. The output vectors are 200-dimensional and are defined for all tokens in the dataset, thanks to the deterministic parsing, for a total of 13 4420 tokens.

Once converted the title and abstract both become variable length sequences of 200-dimensional vectors these are then given to separate bidirectional (Graves et al., 2013) Long Short Term Memory (LSTM) layers (h^1 and g^1) (Hochreiter and Schmidhuber, 1997), the LSTM implementation used is NVIDIA’s cuDNN (Chetlur et al., 2014). These layers each have 256 nodes which then feed to a second set of layer 256 node layers (h^2 and g^2) whose final activations are then combined to produce one 512-dimensional output, this forms the Recurrent Neural Network (RNN) for each of the inputs. The recurrent and LSTM connections are limited to within a layer and do not add to the outputs directly. Finally, outputs from the RNN layers are then combined are then fed into a single fully connected layer (u) that converts the two 512-dimensional outputs into a single 2-dimensional vector giving the log probabilities for each class (\hat{y}).

Figure 3 shows a partially unrolled graph of the complete systems, and Table 3 gives the dimensions. The layers the circular nodes in the figure were all learned via backpropagation. Backpropagation weights updating was done with stochastic gradient descent using and an Adaptive Moment Estimation (ADAM) optimizer (Kingma and Ba, 2014). Due to limitation of the RNN framework a mini-batch size of 1 was the only size available, i.e. after each training sample the weights were updated. For loss the cross entropy was used against a one-hot vector giving the true value, i.e. $[0, 1]^T$ or $[1, 0]^T$.

A 10% random sample of the classified data was taken and used as a validation set with the rest left for training. Since sampling from the training data uniformly has only about a one in five chance of finding a positive example the model would find the local minima of responding negative to all samples. To solve this the positive samples were added to the sample pool twice giving about a one in three chance of being encountered. Then the training was divided into epochs of 500 exposures, after each epoch the testing error and testing loss was computed, these were then used to pick the final model’s number of epochs, as discussed in the next section.

Layer	Description	Operation
Title	Raw title	$string$
Abstract	Raw abstract	$string$
Tokenizer	NLTK <code>word_tokenize</code>	$string \rightarrow \{s_1, s_2, \dots, s_n\}$
Word2Vec	gensim <code>Word2Vec</code> x_t	$s_t \rightarrow \mathbb{R}^{200}$
h^1	forward 256-node $tanh$ activation and LSTM	$\mathbb{R}^{200} \rightarrow \mathbb{R}^{256}$
g^1	reverse 256-node $tanh$ activation and LSTM	$\mathbb{R}^{200} \rightarrow \mathbb{R}^{256}$
h^2	forward 256-node $tanh$ activation and LSTM	$\mathbb{R}^{256} \rightarrow \mathbb{R}^{256}$
h^2	reverse 256-node $tanh$ activation and LSTM	$\mathbb{R}^{256} \rightarrow \mathbb{R}^{256}$
\oplus	Concatenation of final activations	$\mathbb{R}^{256}, \mathbb{R}^{256} \rightarrow \mathbb{R}^{512}$
u	Fully connected linear layer	$\mathbb{R}^{512}, \mathbb{R}^{512} \rightarrow \mathbb{R}^2$
Loss	Cross Entropy Loss	$\mathbb{R}^2, \mathbb{R}^2 \rightarrow \mathbb{R}^1$

Table 3: Specification of the model

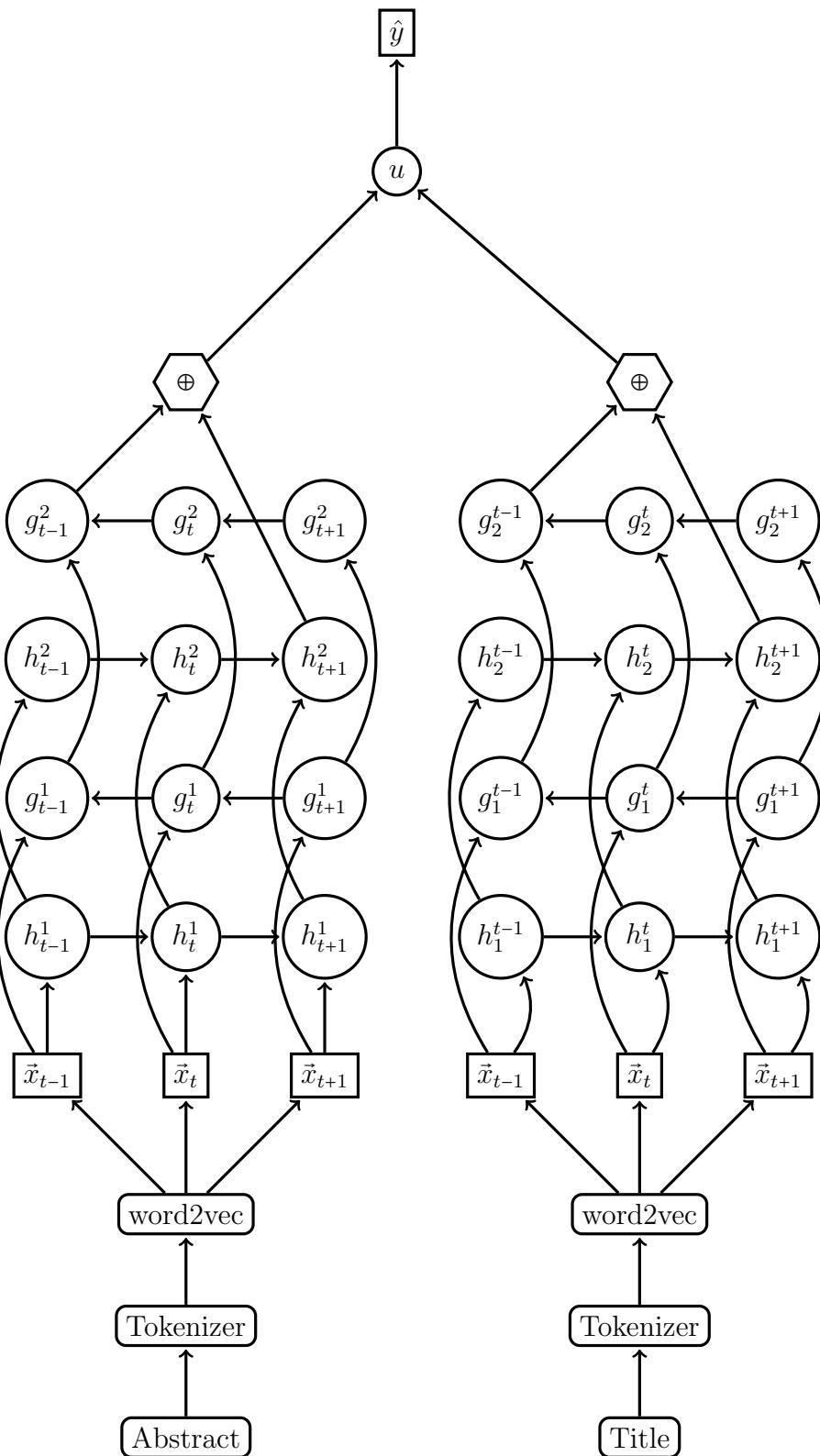


Figure 3: Simplified recursive bidirectional Recursive NN (RNN) layout. LSTM connections were removed for clarity. Circles are NN layers, rectangles with curved corners are the preprocessing, hexagons are combined outputs from the RNN layers, and final output and inputs are indicated with squared corners.

5 Results

When evaluating the model the error rate can be broken into two components, the false positive rate and the false negative rate. Since the positives are sparse the false positive rate can become dominant if too high so it's minimization will have a much large impact than the maximization of the true positive rate (detection rate). Table 5 shows the measured testing statics for 27 epochs (500 exposures of training data per epoch) of training for the data described in Table 4.

Set	Number of Negative	Number of Positive	Percentage Positive
Training	3944	2216	36%
Testing	418	143	25.5%

Table 4: Training-Testing breakdown

Epoch	Loss	Error Rate	Detection Rate	False Positive Rate
0	0.589	0.255	0.000	0.000
1	0.363	0.185	1.000	0.249
2	0.141	0.041	0.916	0.026
3	0.172	0.043	0.937	0.036
4	0.162	0.055	0.965	0.062
5	0.129	0.032	0.944	0.024
6	0.158	0.059	0.958	0.065
7	0.123	0.030	0.937	0.019
8	0.123	0.032	0.958	0.029
9	0.110	0.034	0.923	0.019
10	0.128	0.034	0.944	0.026
11	0.113	0.029	0.944	0.019
12	0.134	0.048	0.972	0.055
13	0.177	0.032	0.895	0.007
14	0.129	0.030	0.916	0.012
15	0.131	0.043	0.881	0.017
16	0.176	0.068	0.944	0.072
17	0.178	0.057	0.951	0.060
18	0.149	0.059	0.846	0.026
19	0.177	0.061	0.811	0.017
20	0.124	0.032	0.923	0.017
21	0.126	0.025	0.951	0.017
22	0.121	0.030	0.909	0.010
23	0.115	0.027	0.937	0.014
24	0.245	0.057	0.832	0.019
25	0.233	0.062	0.790	0.012
26	0.148	0.043	0.860	0.010
27	0.127	0.034	0.916	0.017

Table 5: Testing results per epoch

As the table shows even after a six epochs the testing loss has nearly reached its minima this is fewer exposures than there are examples are in the training data so in theory the training data could be even smaller. As there was no major increase in testing statics to be gained from running training longer and to prevent over-fitting the model used for the rest of the analysis is that from epoch 7. This gives the final model the specification described in table 6.

Epochs	8
Batches per Epoch	500
Testing Loss	0.093
Testing Error Rate	0.023
Detection Rate	0.955
False Positive Rate	0.017

Table 6: Testing results for chosen model

5.1 Model Interpretation

One issue with NN based models is there lack of interpretability, this makes declaring how our trained model works a near intractable problem, particularly for deep architecture like this one. To interpret or visualize the model there are few approaches, first we can embed the samples in a 2-dimensional space via some kind of dimension reduction. In fact since our outputs are 2-dimensional we can just use these. Sadly this does not work as the output variables are highly correlated as shown in figure 4. Also since the data are large texts there is no easy conversion for them into another visualization such as PCA or t-SNE.

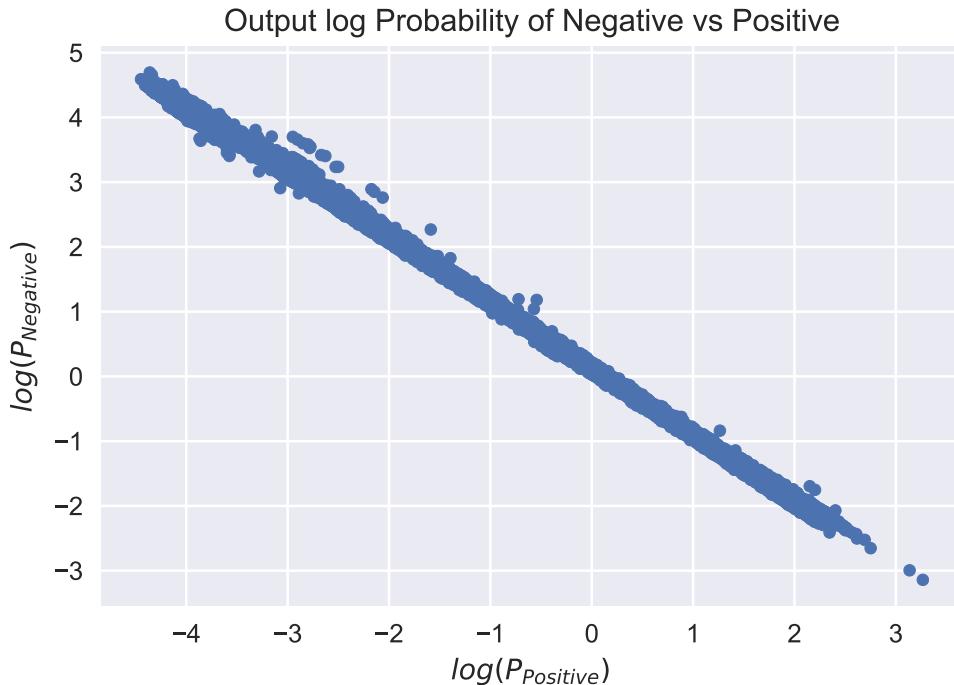


Figure 4: Output for all samples from model

What we can do is examine the activations of the NN layers for a single input. Unfortunately most of the work (Karpathy et al., 2015) in this focuses on the LSTM cells and other intermediate products which are not available to me due to them being on the GPU inside NVIDIA's cuDNN implementation(Chetlur et al., 2014). But what is available are the outputs from the RNN layers. Since all the RNN layer's outputs are the same dimension we can represent them as fixed width heatmaps with red being positive and blue negative and intensity showing magnitude. As an example we will be looking at two input articles a positive article Figure 5 and a negative Figure 6, note only one is from the training set.

Field	Value
ID	WOS:000365978900001
Source	JOURNAL OF STATISTICAL SOFTWARE
Year of Publications	2015
Title	dawai: An R Package for Discriminant Analysis with Additional Information
Abstract	The incorporation of additional information into discriminant rules is receiving increasing attention as the rules including this information perform better than the usual rules. In this paper we introduce an R package called dawai, which provides the functions that allow to define the rules that take into account this additional information expressed in terms of restrictions on the means, to classify the samples and to evaluate the accuracy of the results. Moreover, in this paper we extend the results and definitions given in previous papers (Fernandez, Rueda, and Salvador 2006, Conde, Fernandez, Rueda, and Salvador 2012, Conde, Salvador, Rueda, and Fernandez 2013) to the case of unequal co-variances among the populations, and consequently define the corresponding restricted quadratic discriminant rules. We also define estimators of the accuracy of the rules for the general more than two populations case. The wide range of applications of these procedures is illustrated with two data sets from two different fields, i.e., biology and pattern recognition.
Citation	Conde et al. (2015)

Figure 5: An example of a positive article

Field	Value
ID	WOS:000207446800001
Source	BAYESIAN ANALYSIS
Year of Publications	2006
Title	When Did Bayesian Inference Become "Bayesian"?
Abstract	While Bayes' theorem has a 250-year history, and the method of inverse probability that flowed from it dominated statistical thinking into the twentieth century, the adjective "Bayesian" was not part of the statistical lexicon until relatively recently. This paper provides an overview of key Bayesian developments, beginning with Bayes' posthumously published 1763 paper and continuing up through approximately 1970, including the period of time when "Bayesian" emerged as the label of choice for those who advocated Bayesian methods.
Citation	Fienberg et al. (2006)

Figure 6: An example of a negative article

You should be able to tell from reading the titles of each article if they introduce a new software package and so to it seems can the model. Figure 7 shows the activations of the outer layers g^2 and h^2 at each word. The top figure is for the positive example, the middle for the negative and bottom a comparison of their final outputs. Since only the final outputs are used by the fully connected layer and thus learned with backpropagation they are much more significant than their predecessors. But the outputs of the penultimate and latter words can still be considered to be approximations of the final outputs since the RNN does not know if a word is the last.

By making this reasonable assumption we can further infer that the outputs are being updated as the RNN moves through the text, note the RNN reads it both forward and reverse once. Thus we can interpret each words activations as a description of the text up to that point, e.g. after each word the RNN describes what it has seen in a way the fully connected layer can understand.

Determining what each of the 512-dimensions means is a fool's errand since some may have no meaning and some might be combined with others in complex ways. But we can consider the broader picture and look for transitions and differences. Both the title, Figure 7, and abstract, Figure 8, have a couple strongly dissimilar values in their final outputs. This suggested these are dimensions representing major differences in their contents and by looking at many other examples I can see that some of these differences are present in all such comparisons implying they represent votes from the RNN layer as to the classification of the input.

Another phenomenon shown in the both diagrams is regions of high activation, most notably the top example in Figure 8 only has the normal levels in the last few words. My interpretation of this is it is the RNN displaying uncertainty. in Figure 8 the activations for the word ‘*package*’ are very different than the word ‘*Discriminant*’. This is because a title with the word ‘*package*’ in it is very likely to be a new software package while ‘*Discriminant*’ is the reverse, thus reading ‘*Discriminant*’ after ‘*package*’ causes the RNN’s description to shift towards negative, while a word like ‘*Additional*’ has no such significance and thus no effect.

What is interesting is that the uncertainty is expressed as an increase in density, this can be better explained by looking at Figure 8. For both articles the initial state of the output is dense, this gives much more bandwidth than the final quite sparse outputs. This increase in bandwidth gives the fully connected layer more much more information and thus it can compose a much more complicated combination of both the title and abstract RNNs. Thus when an RNN is certain in its results it outputs a sparse set of weights e.g. a short message while when uncertain it returns a much longer one. This makes sense intuitively, if asked to describe a car to someone if you recognize the make and model your description might just be that while if you did not you would have to describe each component separately.

Further analysis of these activations is merited but beyond the scope of this report. But from these I can confidently say that the model is reading and understanding the text at a level of complexity greatly exceeding a simple regex or SVM.

5.2 Output

The output from the model is a 2-dimensional vector with the first dimension being the log probability of the input being negative and the second the log probability of it being positive. There is no guarantee that the probabilities sum to 1, but as Figure 4 shows the probabilities are mostly symmetric. Thus to get a classification from the model we can simply look at the highest values say that is the classification. When we do this across the entire data set we get the results shown in Table 7 for each year.

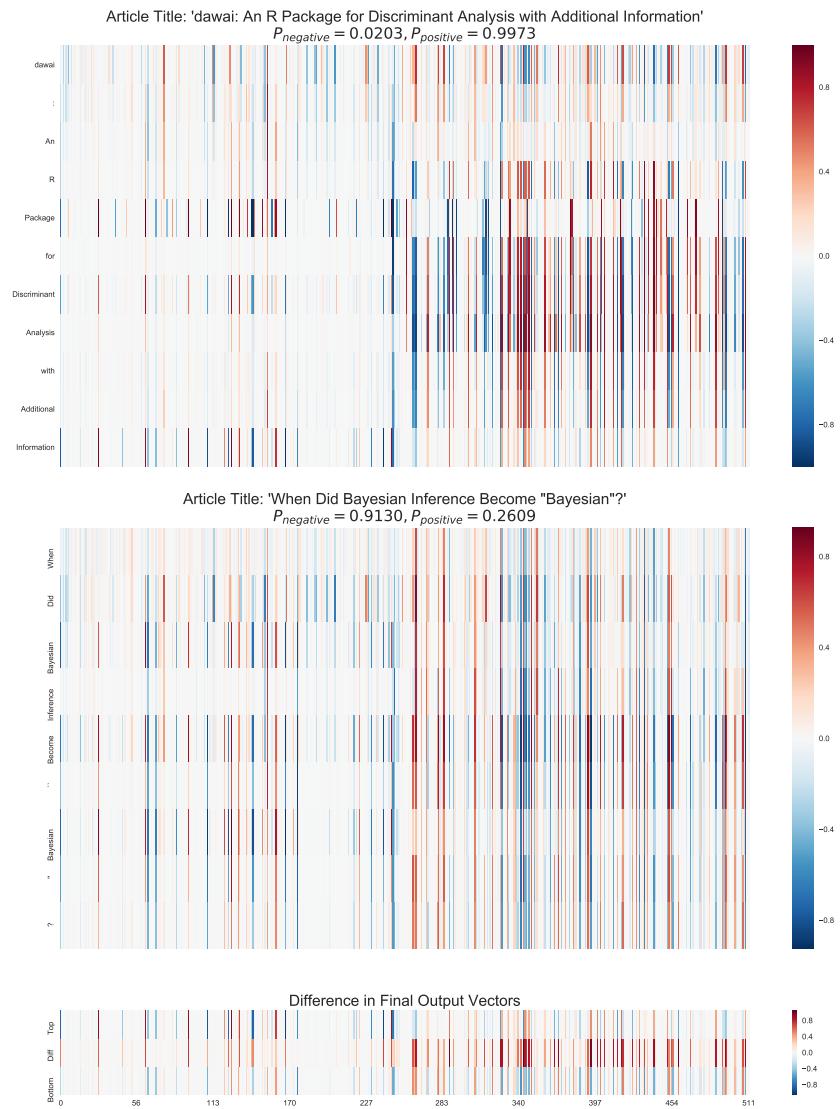


Figure 7: RNN activations for each word in two titles; the positive example is on top, the negative below it, and a comparison of each input's final output is shown at the bottom.

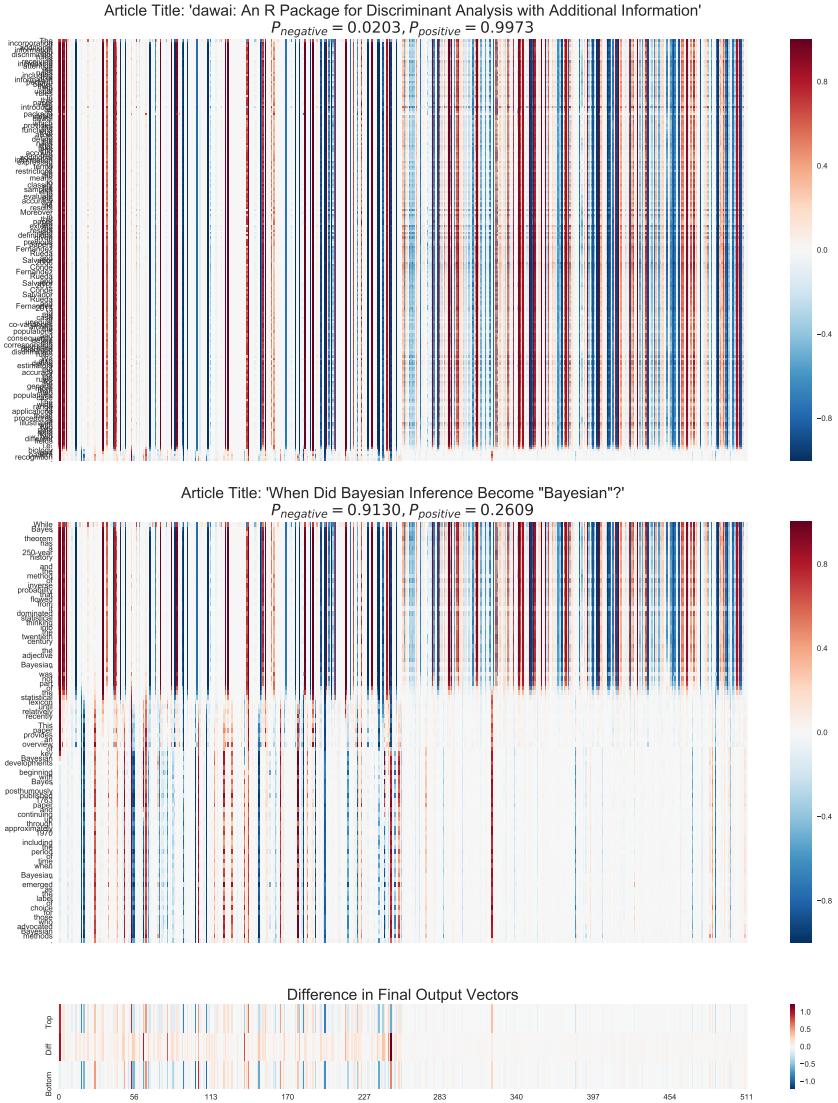


Figure 8: RNN activations for each word in two abstracts; the positive example is on top, the negative below it, and a comparison of each input's final output is shown at the bottom.

Year	Number of Articles	Not Software	Software	New Software Percentage
2005	5 235	4 998	237	4.52%
2006	5 806	5 522	284	4.89%
2007	6 255	5 914	341	5.45%
2008	7 085	6 703	382	5.39%
2009	7 435	7 047	388	5.21%
2010	7 216	6 801	415	5.75%
2011	7 767	7 280	487	6.27%
2012	7 990	7 519	471	5.89%
2013	8 287	7 829	458	5.52%
2014	8 336	7 830	506	6.07%
2015	7 559	7 095	464	6.13%
Total	78 971	74 538	4433	5.61%

Table 7: Per year result across all papers

Table 8 shows the top journals by counts, while Figure 9 shows each journal's software and non-software counts.

Class	Count	Journal
Highest software count (Training)	673	JOURNAL OF STATISTICAL SOFTWARE
Highest software count (Non-training)	171	IEEE-ACM TRANSACTIONS ON COMPUTATIONAL BIOLOGY AND BIOINFORMATICS
Highest non-software count (Training)	1 156	ANNALS OF STATISTICS
Highest non-software count (Non-training)	3 381	STATISTICS & PROBABILITY LETTERS

Table 8: Top journals for each class in training and full dataset

We can also break down the counts per language, as in Table 9. These counts are derived from a very simple sub-string search and as such can not be considered to be very accurate, they are likely under counting most categories. But they do show that the expected result of R being by far the most popular. Interestingly one of the most popular languages JavaScript has no representation.

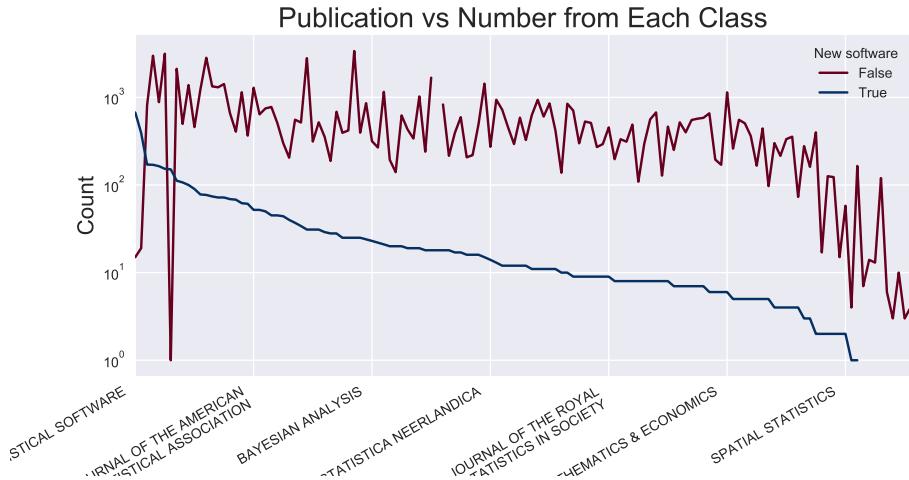


Figure 9: Counts for each class against each journal, ordered by number of positive examples, note y axis is log

Language	count
R	566
Stata	130
Matlab	37
SAS	32
C	12
Mathematica	7
Python	6
Java	3
SPSS	1
C++	1
JavaScript	0
Perl	0

Table 9: Per language counts for from positive examples

6 Discussion

As I have shown, the model is capable of identifying complex ideas in textual data. The training set is both relatively small and imperfect; in fact, when the false classifications are examined by an expert, most of them result from errors in the data and not in the model. Thus, by using the model to help generate cleaner

data, a new model could be trained with higher accuracy. The main issue is the false detection rate, which could be reduced by training a cascade of NNs instead of a single one.

These issues aside, the research undertaken herein demonstrates large-scale detection of new software introduced in scientific literature. We can use this data to start making inferences about the usage of software by statisticians. First we can see that a large number of them likely use a programming language or software tool if 5.6% of all papers are statisticians creating new tools if even five other papers use the tool then 30% of all papers would have some computational aspect and this is likely greatly understanding the diffusion. We can also see that usage is rising, with 2005 having 1% less usage than 2015, this is likely due to computational methods becoming more important in the last decade. What is also shown is that computational methods are not clustered in one or two journals, most for most journals there is a 1–4% chance of a random article being a new software tool. This means that most statisticians are reading about computational tools and thus are likely using them. Finally we can see that to no ones surprise R is by far the most dominant language for statisticians.

The next steps are to do biometric and natural language processing on our corpora as there are many questions we can answer. Of interest to us are '*How programming languages distributed across the sciences?*', '*What properties of new scientific software packages cause them to be accepted by a community?*' and '*What is the relationship between success as an article and success as a software tool?*'. All of these questions are important to understanding how software has shaped the way scientists work and how scientists have shaped their tools.

The question most pressing to me is '*What properties of new scientific software packages cause them to be accepted by a community?*' to answer this I would study the activation plots like those in the interpretation section, to find those activations that correspond to the naming of the package and to the naming of the language. These both should exist as they are some of the strongest indicators of a positive sample. From this I can lookup the source code of the package as well as a variety of other pieces of information including if available their entry in repository. This then would let me link WOS ID numbers to software packages at a large scale and from that I can analyse the biometrics of the package. This would let me look for patterns in usage across both the scientific domain and the repository level.

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