Towards Math-Aware Automated Classification and Similarity Search of Scientific Publications

Methods of Mathematical Content Representations

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Abstract. In this paper, we investigate mathematical content representations suitable for the automated classification of and the similarity search in STEM documents using standard machine learning algorithms: the Latent Dirichlet Allocation (LDA) and the Latent Semantic Indexing (LSI).

The methods are evaluated on a subset of arXiv.org papers with the Mathematics Subject Classification (MSC) as a reference classification and using the standard precision/recall/F$_1$-measure metrics. The results give insight how different math representations may influence performance of the classification and similarity search tasks in STEM repositories. Non-surprisingly, machine learning methods are able to grab distributional semantics from textual tokens. A proper selection of weighted tokens representing math may improve the quality of the results slightly. A structured math representation that imitates successful text-processing techniques with math is shown to yield better results than flat TeX tokens.

1 Introduction

There are many machine learning techniques usable for the automatic classification. [14] Historically, the bag of words (BoW) technique was used with metadata and full texts. Papers from the Science, Technology, Engineering, and Mathematics (STEM) domain are specific in the massive use of mathematical expressions. However, these parts of documents were usually omitted altogether even though they may be highly important for the proper document representation. It was shown, for example, that the performance of classifiers depends even on the semantic drift of concepts in a language over time. [13] Watt [17] has shown that even a sole histogram of mathematical symbols that were used in a paper is sufficient for a rough classification of scientific papers into mathematical subdomains.

In this paper, we investigate the usefulness of various representations of mathematical content (see Section [2] for the automated classification of and the similarity search in STEM documents using machine learning algorithms. We use
a human-assigned MSC (see Section 3) as a reference for measuring the quality of the results. In Section 5, this known classification is used as a reference for evaluating the results of processing various document representations specified in Section 4 with different setups of the Latent Dirichlet Allocation (LDA) and the Latent Semantic Indexing (LSI) machine learning algorithms. To evaluate the results, we use the standard metrics: precision, recall and the micro F1-measure in Section 6. Results are discussed in Section 7 followed by conclusions in Section 8.

2 STEM Document Representations

The transformation of a text document to a BoW is often more complex than splitting the text to individual word tokens. It is necessary to cope with punctuation, to ‘normalize’ the words transforming all characters to lowercase, to apply stemming or lemmatisation, etc. These text-processing techniques are well established, but the processing and the representation of mathematical content have not yet been properly explored. For expressing math TEX markup is used on the authoring side, and MathML for web document exchange. When indexing documents with math for search, many representations have been explored and used. The markup varies from presentation to content/semantic one, with prevalence availability of presentation notation, available as a common denominator of conversions from different primary document formats.

We experimented with two different math statement representations:

TEX Compact linear plain text TEX notation is well known to the authors of STEM documents. The vast majority of papers in math is authored in the TEX markup.

For example the TEX representation of the simple formula $a + b^{2 + c}$ is:

\[ a + b^{2 + c} \]

MTerms The MTerms are a special compressed and generalized encoding of formulae based on the original MathML representation of math in our data corpus.

For example, the MTerm representation of the simple formula $a + b^{2 + c}$ is:

\[ R(I(a)O(+)J(I(b)R(N(2)O(+)I(c)))) \]

MTerms, described in [15, p. 233], were developed as an internal math formulae representation of the math-aware full text search system MIaS. [15, p. 234 bottom]

An important feature of MIaS MTerms processing is the canonicalization of mathematical content [6] that is incorporated in the MTerms derivation process. The canonicalization ensures that identical terms can be found in distinct documents sharing not just identical, but also only similar subcomponents of otherwise distinct complex formulae.

Another important feature of the MIaS implementation is the ability to derive multiple MTerms from a single input formula. [16] These additional MTerms represent subformulae (subcomponents) of the original formula and their generalized (unified) variants with variables and constants substituted with general identifiers. See Figure 1.
Fig. 1: An example of formula preprocessing inside the MIaS system. During the processing, the order of components in the formula is normalized and subformulae are derived. The last two steps of the processing add generalized forms of all the (sub)formulae with variables and constants unified to generalized identifiers. For more details, see [16]. Derived components have a derived MIaS weight assigned, reflecting the degree of change compared to the original formula. All these components starting at the ordering level are consequently converted to the MTerm encoding and provided together with the particular MIaS weights as weighted MTerms.

To reflect differences between the top-MTerms, i.e. MTerms representing the original formulae from the dataset (i.e. the formula \(a + b^2\) in Figure 1), and derived-MTerms representing the derived forms of these formulae (the formulae at the lower levels of the processing tree in Figure 1), the MIaS system assigns a MIaS weight \(\in (0,1) \subset \mathbb{R}\) to both top- and derived-MTerms. The MIaS weight reflects the distance of a particular MTerm from the original formula. The lower the weight, the greater the distance. Weighted MTerms are tuples of the MTerm and its MIaS weight, i.e.:

\[
\text{\{ "mias_weight" : 0.125,}
\text{ "mterm" : "R(I(a)O(+)J(I(b)R(I(c)O(+)N(2))))" \}}
\]

in the case of the top-MTerm representing formula \(a + b^2\) in Figure 1.

To sum things up, the MTerms representation covers not only the original formulae but also a variety of its derivatives.

1 Please note, however, the top-MTerm weight is not 1.0. The initial weight of the formula is computed based on the number of subcomponents of the formula. See Figure 1 for more details see [16].
We exploited the existing implementation of the formulae normalization and
decomposition in the MIaS to imitate some successful text-processing techniques
(such as the normalization of word forms) with formulae. We tested various
strategies for selecting MTerms from the dataset. MTerms and the \text{T\LaTeX} statements
alone were used as the final tokens without any further processing.

3 Dataset

In our experiments, we used the \text{arXiv.org} STEM articles with known MSC
codes \cite{2} as a reference classification. Their original \text{T\LaTeX} format is hard to fully
process without a full-featured \text{T\LaTeX} compiler, so we used the NTCIR-11 Math-2
dataset\cite[2, p.89]{1} of 105,120 scientific articles from arXiv.org. The articles in the
dataset were converted to the XML-based XHTML5 format with mathematical
formulae converted to MathML annotated with \text{T\LaTeX}.

We selected 8,004 articles from our dataset with exactly one MSC assigned.
Since they are assigned by the document authors themselves, we assume that the
MSC codes are valid and that they match the document content. Out of these
documents, we selected those with ‘good’ MSC codes in which the third character
of a code was \textit{neither} - (hyphen) \textit{nor} . (period) and the MSC specification
available \cite{2} did \textit{not} contain any ‘see also’ references to other MSC codes. The
aim of this filtering was to have correct reference data excluding ‘weakly defined’
codes. The assignment of exactly one primary MSC code to a document indicates
that the document content fits well enough to exactly one MSC category to be
used as a reference representation of the category.

5,619 articles from our dataset met all these criteria and were used as a data
corpus for our experiments.

4 Data Preprocessing and Document Representation

All documents were transformed from the XHTML5 format to an internal repre-
sentation consisting of:

\textbf{metadata} the basic document metadata such as the unique document ID, the
MSC classification, the title, the authors, and the abstract,
\textbf{text} the plain-text representation of the full text of the document with all math
formulae removed, and
\textbf{math} the math formulae in the \text{T\LaTeX} and MTerms formats (see Section \cite{2}).

All token types (text, \text{T\LaTeX}, and MTerms) used in a particular experimental
setup were put to a single common BoW. Math tokens were prefixed and suffixed
with a single $ character to keep even trivial tokens such as a variable $a$ (resulting
in the token $a$) distinct from the text word ‘a’ (resulting in the token a).

\footnote{The dataset is available free of charge for research purposes:\url{http://research.nii.ac.jp/ntcir/permission/ntcir-11/perm-en-MATH.html}}
Text elements were tokenized using the Unitok tool. Segmentation to sentences was not performed and instead all tokens across all sentences were merged into a single flat BoW.

In some of our experimental setups, we selected only a subset of the available MTerms based on their final weights. The final weight $\text{weight}_{\text{token}}$ of a particular MTerm token was computed as follows:

$$\text{weight}_{\text{token}} = \lceil \text{round}(\text{MTermWghtMod}(\text{mias_weight})) \rceil,$$

where $\text{mias_weight}$ is the MIaS weight of the MTerm and $\text{MTermWghtMod}()$ is a function whose definition varies across the experimental setups. A particular MTerm was added $\text{weight}_{\text{token}}$ times to the BoW.

5 Algorithms

For our experiments, we used Gensim [12], a popular state-of-the-art vector space and topic modelling toolkit. In particular, we were comparing the vector space model transformation of BoW on various representations of the input data using the Latent Semantic Indexing (LSI) [5] and the Latent Dirichlet Allocation (LDA) [4] transformations both with and without the Term Frequency–Inverse Document Frequency transformation [11] (TfIdf-LSI, TfIdf-LDA). The input data were indexed for cosine measure document similarity queries using the \texttt{gensim.similarities.docsim.Similarity} interface of Gensim.

The input formulae are occasionally very long. To reduce the dictionary size, math tokens longer than their hex string representation in MD4 were replaced with their MD4 hashes.

6 Evaluation Setup

We exploit the known MSC of the documents in our dataset as a reference classification for our evaluation. An MSC code being assigned to a document signifies that the topic (content) of the document is similar to other documents with the same MSC code assigned. Thus, we expect that a suitable setup of the machine learning methods should distribute documents with similar content to groups of similar documents that will correspond to the grouping induced by the MSC classes.

The machine learning process on our dataset results in a number $s \in (0, 1) \subset \mathbb{R}$ for every pair of documents from the testing corpus, expressing the mutual similarity of the two documents. The higher the number is, the more similar the two documents are.

As such, the results can be expressed as a matrix where every column/row belongs to one article from the testing corpus. Articles in columns/rows of the matrix are ordered according to their MSC code. See Figure 2. Value $s_{i,j}$, i.e. the value in the row $i$ and the column $j$ of the matrix, expresses the mutual similarity value of the $i$-th and the $j$-th document according to their MSC ordering. As the
Fig. 2: The similarity matrix schema. The thin grid represents borders between individual articles, the thick grid represents borders between MSC regions (groups of articles in different MSC top-level categories), and gray squares represent the MSC regions grouping the similarity values of articles with identical MSC top-level categories.

documents are ordered according to their MSC codes from left to right and from top to bottom, the main diagonal of the matrix represents the similarity of every document with itself.

We visualized the similarity matrices resulting from our experiments as grayscale images, transforming the similarity values \( s_{i,j} \) to \( \{0, \ldots, 255\} \subset \mathbb{Z} \); this value represents the brightness of the pixel in the images. To make the image more readable, the transformation was not linear but logarithmic to make highly similar pairs of articles more visible as bright pixels in the image. Completely white lines represent borders between MSC top-level category regions, i.e. groups of articles in different MSC top-level categories; these categories are specified by the first two letters of an MSC code. See Figure 3a.

The optimal classification method will produce white squares in the MSC regions on the main diagonal, indicating high similarity between the articles belonging to the same MSC top-level category, and black rectangles in the MSC regions everywhere else, indicating low similarity between articles from different MSC top-level categories. Unsuccessful classification method does not produce these structures in the image; cf. Figure 3a and 3b. We will use this observation to rigorously evaluate the quality of results from all experimental setups using the standard precision/recall and the F\(_1\)-measure metrics. [7]

To compute these metrics, we need a reference perfect similarity matrix that defines the optimal classification result. This matrix has the similarity value of 1 for all items inside the MSC regions on the main diagonal and 0 everywhere else. Figure 2 shows such a perfect similarity matrix with the gray areas representing 1s and the white areas representing 0s.
(a) A successful experimental setup (configuration #11 in Table 1).
(b) An unsuccessful experimental setup (configuration #6 in Table 1).

Fig. 3: A visualization of real similarity matrices from selected results. Bright pixels represent the mutual similarity of a pair of MSC-ordered documents at given a row/column; the more bright the pixel, the more similar the two documents are. Completely white horizontal/vertical lines represent borders between the MSC top-level category regions. The magnified circular area in Subfigure 3a shows a sharply bounded subcategory in the region for the top-level MSC code of 68 (Computer Science); this subcategory was automatically detected by the machine learning method.

To compute precision/recall and consequently the F_1-measure, we need to select a threshold $t$ for the transformation of the similarity value $s$ to $s' \in \{1, 0\} \subset Z$ such that $s' = 1$ if $s \geq t$ and $s' = 0$ otherwise. In our experiments, we evaluated the results for a large number of samples of $t$ values across its possible interval to see the precision/recall/F_1-measure curve shape for different $t$ values. To compare results of different experimental setups we used results for $t$ at precision/recall intersection of the particular result.

Using the matrix schema in Figure 2 the gray areas are the relevant items, whereas the white areas are the irrelevant items. The values of $s'_{i,j} = 1$ are then true positives inside the gray areas and false positive inside the white areas; conversely, the values of $s'_{i,j} = 0$ are true negatives inside the white areas and false negatives inside the gray areas for the precision/recall computation.

Scikit-learn [10] was used to compute precision ($p$) and recall ($r$) using `sklearn.metrics.precision_recall_curve`. Consequently, the F_1-measure in the micro variant is computed at the given similarity threshold as $F_1 = \frac{2pr}{p+r}$. See the example in Figure 4.

Prior to the evaluation, we prepared a randomly ordered list of all available documents. The randomization was done only once at the beginning to have a selection that is random but that also stays stable over the course of all experiments. Evaluation was done using the k-fold cross-validation method [9].
with \( k = 2 \), where one fold of the randomly sorted documents was used to train the model and the rest was used as a testing corpus. 63 top-level MSC categories were present with an average of 44 documents per category and a median of 19 documents per category. To further improve the accuracy of the results (LDA is a probabilistic method) the \( k \)-fold cross-validation was run 4 times for every experimental setup. Consequently, the arithmetic mean and the variance of all values were computed and used.

7 Discussion of Results

The basic set of results is shown in Table 1. The table is sorted according to the \( F_1 \)-measure (micro). For every setup, the threshold was automatically determined to be the break-even point at which precision equals recall. In addition, the maximum \( F_1 \)-measure (micro) reachable for each of the results by adjusting the similarity threshold is shown.

2-fold cross-validation with 4 reruns was used to validate the results. The arithmetic means of the metrics over all the runs are shown in the ‘(avg)’ columns, a good stability of the method is indicated by the low variances shown in ‘(var)’ columns. The best result using text/TEX/MTerms only are highlighted in bold. Configuration #11 can be considered as the baseline as it represents the best result using only text contents of the documents with no involvement of mathematical formulae.
Table 1: Experiments uses 50 topics and the 2-fold cross-validation with 4 reruns. For the LDA algorithm, gamma_threshold=0.001, 10 iterations and 10 passes were used. When top/high/mid/low-MTerms used every MTerm was added exactly once to BoW. Data are sorted according to the $F_1$-measure (micro) for similarity threshold at precision/recall intersection.

| Config # | TEX | MTerm | Text | Method | $F_1$ micro at P/R inters. (avg) | $F_1$ micro at P/R inters. (var) | Maximal $F_1$ micro (avg) | Maximal $F_1$ micro (var) |
|----------|-----|-------|------|--------|--------------------------------|-------------------------------|--------------------------|----------------------------|
| 115       | -   | -     | +    | TfIdf-LSI | 0.3427                          | 0.0000                        | 0.3431                   | 0.0000                     |
| 11        | -   | -     | +    | TfIdf-LSI | 0.3419                          | 0.0000                        | 0.3425                   | 0.0000                     |
| 15        | +   | -     | +    | TfIdf-LSI | 0.3366                          | 0.0000                        | 0.3369                   | 0.0000                     |
| 8         | -   | -     | +    | LDA    | 0.3331                          | 0.0003                        | 0.3356                   | 0.0003                     |
| 9         | -   | -     | +    | LSI    | 0.2847                          | 0.0000                        | 0.2876                   | 0.0000                     |
| 12        | +   | -     | +    | LDA    | 0.2523                          | 0.0003                        | 0.2603                   | 0.0002                     |
| 303       | low | +     | -    | TfIdf-LSI | 0.2446                          | 0.0000                        | 0.2478                   | 0.0000                     |
| 203       | high| +     | -    | TfIdf-LSI | 0.1922                          | 0.0001                        | 0.1968                   | 0.0001                     |
| 403       | mid | +     | -    | TfIdf-LSI | 0.1913                          | 0.0000                        | 0.1979                   | 0.0000                     |
| 24        | +   | +     | +    | LDA    | 0.1837                          | 0.0000                        | 0.1922                   | 0.0000                     |
| 28        | +   | +     | +    | LDA    | 0.1805                          | 0.0001                        | 0.1893                   | 0.0000                     |
| 16        | -   | +     | +    | LDA    | 0.1743                          | 0.0002                        | 0.1847                   | 0.0001                     |
| 20        | +   | +     | -    | LDA    | 0.1741                          | 0.0001                        | 0.1839                   | 0.0000                     |
| 111       | -   | top   | -    | TfIdf-LSI | 0.1568                          | 0.0000                        | 0.1632                   | 0.0000                     |
| 27        | -   | +     | +    | TfIdf-LSI | 0.1535                          | 0.0000                        | 0.1614                   | 0.0000                     |
| 19        | -   | +     | -    | TfIdf-LSI | 0.1533                          | 0.0000                        | 0.1612                   | 0.0000                     |
| 23        | +   | +     | -    | TfIdf-LSI | 0.1532                          | 0.0000                        | 0.1613                   | 0.0000                     |
| 31        | +   | +     | -    | TfIdf-LSI | 0.1528                          | 0.0000                        | 0.1610                   | 0.0000                     |
| 202       | high| -     | +    | TfIdf-LSI | 0.1486                          | 0.0000                        | 0.1562                   | 0.0000                     |
| 7         | +   | -     | -    | TfIdf-LSI | 0.1392                          | 0.0000                        | 0.1512                   | 0.0000                     |
| 4         | +   | -     | -    | LDA    | 0.1375                          | 0.0001                        | 0.1480                   | 0.0000                     |
| 302       | low | +     | -    | TfIdf-LSI | 0.1344                          | 0.0000                        | 0.1453                   | 0.0000                     |
| 402       | mid | -     | -    | TfIdf-LSI | 0.1264                          | 0.0000                        | 0.1395                   | 0.0000                     |
| 5         | +   | -     | -    | LSI    | 0.1181                          | 0.0000                        | 0.1343                   | 0.0000                     |
| 10        | -   | -     | +    | TfIdf-LDA | 0.0888                          | 0.0001                        | 0.1092                   | 0.0001                     |
| 22        | +   | +     | -    | TfIdf-LDA | 0.0664                          | 0.0000                        | 0.0898                   | 0.0000                     |
| 18        | -   | +     | -    | TfIdf-LDA | 0.0657                          | 0.0000                        | 0.0892                   | 0.0000                     |
| 26        | -   | +     | +    | TfIdf-LDA | 0.0655                          | 0.0000                        | 0.0881                   | 0.0000                     |
| 29        | +   | +     | -    | LSI    | 0.0654                          | 0.0000                        | 0.0910                   | 0.0000                     |
| 30        | +   | +     | +    | TfIdf-LDA | 0.0643                          | 0.0000                        | 0.0875                   | 0.0000                     |
| 6         | +   | -     | -    | TfIdf-LDA | 0.0589                          | 0.0000                        | 0.0850                   | 0.0000                     |
Fig. 5: Precision/recall curves of one of the tested MTerms content representations (configuration #16 in Table I)

7.1 Properties of the Evaluation Method

We evaluate our results against ‘the perfect MSC similarity matrix’ (see Section 6)—an idealized model that expects all the documents belonging to the same top-level MSC category to be perfectly similar and completely dissimilar to documents in the remaining top-level MSC categories. In reality, we cannot expect sharp contrast in the used terminology or even in the general mathematical notation.

Nevertheless, Figure 3a shows numerous bright sub-regions of highly similar articles inside the top-level category regions along the main diagonal. Quite sharply bounded is a sub-square of bright pixels, magnified in the image, within the region for the top-level MSC code of 68 (Computer Science). These indicate the successful determination of MSC subcategories showing that the classification method is capable of fine-grained classification not reflected in our idealized reference model.

Thus, the absolute values of the F_1 that we reached are of less importance for the interpretation of our results. The relative differences between the various content representations are more important for us to determine the usefulness of math content for machine learning.

7.2 Exclusive use of text/TEX/MTerms

The best results using only text/TEX/MTerms are highlighted in bold. Configuration #11 can be considered the baseline, as it represents the best result using only text content of the documents with no involvement of mathematical formulae.

The table shows that the exclusive use of mathematical content in either TEX or MTerms form cannot supersede the text representation: the F_1-measure at
the precision/recall intersection (hereinafter referred to as $F_1$) 0.1392 for TP\$X
and 0.1743 for MTerms are significantly lower than the 0.3419 for the text.

However, it is important to keep in mind that the tested methods are
unsupervised—we did not provide the system with any hints on the expected
classification. Consequently, the difference in text and math content performance
may indicate that (textual) terminology varies more between different MSC areas
than math notation does and therefore the text content is more suitable for the
task of determining the top-level MSC category. This interpretation is supported
by the observation of a decrease in the $F_1$ of the text representation after adding
unfiltered math content (see the difference between configurations #11 and #15
or between #8 and #28 in Table 1)—math, less suitable for this particular task,
adds noise, decreasing the quality of the classification.

7.3 Comparison of Machine Learning Methods

**TfIdf-LSI** worked best with the combination of text and top-MTerms represen-
tations (#115 in Table 1).

**LDA** follows closely with the text only representation.

**LSI** follows the LDA setup with a decrease of 15% in terms of $F_1$ with the text
only representation.

**TfIdf-LDA** yielded poor results in general; $F_1 < 0.1$ in the average case.

For LDA, tuning the gamma threshold (values 0.1, 0.01, and 0.001) and the
number of iterations (values 10 and 100) had a minimal impact on the results. In
terms of $F_1$, the difference was less than 0.006 for each parameter with otherwise
identical setups.

TfIdf-LSI has shown the best performance; we will therefore concentrate on
this method in the next section.

7.4 Impact of the Number of Topics

To test the hypothesis that the worse overall performance of math over text
content is caused by the low number of topics (50 topics were used in most setups)
limiting the rich structure of math formulae to a small subset, we used a batch
of configurations with 100, 500, 1,000 and 5,000 topics.

Using TfIdf-LSI, the higher number of topics led to a worse performance
using text only: $F_1$ decreased from 0.3340 for 100 topics to 0.3021 for 5,000
topics. For MTerms or a combination of MTerms with text, the difference in $F_1$
was negligible (0.01), although marginally better results were achieved with 500
topics.

Thus, the low number of topics does not seem to limit performance using
math representations.
7.5 Selection of MTerms

An important feature the MTerms mathematical content representation has, unlike the TeX format, is the normalization of formulae and the derivation of subformulae (see Section 2). A single input formula is converted to a set of weighted MTerms and we may choose to select only a subset of the MTerms for the machine learning procedure.

In most experimental setups, we used MTerms filtered according to their weights modified with the following definition of `MTermWghtMod()` in Python: `trunc(390 * mias_weight)` (see Section 4). This definition is the result of our initial analysis of the MIaS subformulae weighting [16] and experimental runs aimed to include only the original formulae and their first-level derivatives. The final weight `weight_token` of a particular MTerm token is reflected in the BoW by adding the MTerm token `weight_token`-times.

We also tested an alternative method of MTerm selection with the TfIdf-LSI approach. Every MTerm was considered for inclusion in BoW according to the MIaS weight. If the MTerm was selected for inclusion, then it was added to the BoW exactly once regardless of its MIaS weight.

We tested multiple selection strategies:

**Top-MTerms** This strategy selects only top-MTerms, i.e. MTerms representing the original formulae from the dataset after ordering the canonicalizing the elements (see Section 2).

**High-MTerms** This strategy selects only one third of the highest-weighted MTerms out of the formula set.

**Mid-MTerms** This strategy selects only one third of the middle-weighted MTerms out of the formula set.

**Low-MTerms** This strategy selects only one third of the lowest-weighted MTerms.

Similarly to the full MTerms set, the selected MTerm strategies reached overall higher scores when combined with texts.

However, the exclusive use of top-MTerms (#111 in Table 1) reaches $F_1$ of 0.1568, i.e. performs better than exclusive use the full set of the weighted MTerms (#19 that reached $F_1$ of 0.1533). The exclusive use of high-/low-/mid-MTerms (#202, #302, #402) follows with the $F_1$ scores of 0.1486/0.1344/0.1264. The fact that middle-weighted MTerms score lower than both high- and low-MTerms might indicate that the MSC category is better determined using full-length formulae (high-MTerms) or the extracted basic elements of formulae such as specific symbols (low-MTerms) than using the common notation ‘in the middle’ (mid-MTerms).

Using a combination of high-/low-/mid-MTerms with text (#203, #303, #403) confirms mid-MTerms to be less useful (reaching $F_1$ of 0.1913). However, low-MTerms reaching $F_1$ of 0.2446 work clearly better than high-MTerms reaching $F_1$ of 0.1922 in this case.

The most interesting setup is the combination of top-MTerms with the text. This setup (#115 in Table 1) reached $F_1$ of 0.3427, the highest out of all of
our experimental setups, yielding marginally better results than both the text
only configuration #11 (F₁ 0.3419) and combination of text and \TeX\ (#15, F₁
0.3366).

8 Conclusions

The aim of this paper was to investigate mathematical content representations
for machine learning algorithms. These representations were chosen to be suitable
for the automated classification of and the similarity search in STEM documents.
We tested on a dataset of arXiv.org papers with a known MSC. This classification
was consequently used as the reference classification for the evaluation of various
setups of our unsupervised machine learning procedure.

For mathematical content representation, we used two distinct formats: un-
structured \TeX\ representation and the normalized and generalized weighted
complex structural representation of MTerms.

For our task of an unsupervised classification of STEM papers according to
the MSC, the text content representation with top-MTerms works best (F₁ of
0.3427) but with only very small margin to the exclusive use of text (F₁ of 0.3419)
or the combination of text and \TeX\ (F₁ of 0.3366).

Exclusive use of text (F₁ 0.3419) works better than exclusive use of MTerms
(F₁ of 0.1744) or \TeX\ (F₁ of 0.1392). However, this may only indicate that textual
terminology varies more between different MSC areas than math notation and as
such, text content is more suitable for the determination of MSC.

Even though we did not reach a clear improvement with the use of math
content, the combination of text and math still achieved the highest score in our
experiments. According to our results, this is due to the proper selection of math
representants – the canonicalized top-MTerms.

This leads us to believe that mathematical content has its use in the machine
learning of the similarity of STEM papers. However, to have a positive impact, the
proper selection of a small number of math content representants is needed. We
believe that thoroughly selected math tokens added to the text tokens can refine
the final similarity score in the corner cases where the limits of distinguishing
based on text content alone are reached. For example, in the case of highly formal
mathematical articles, the high percentage of the overall content are formulae
and text only act as a ‘glue’. Because of that, there are then few specific text
keywords and the importance of the formulae for assigning the correct similarity
score is high.

However, as discussed in Section 7.1 we evaluate against an idealized model
on top-level MSC categories. We assume the positive effect of properly selected
math content representants on the corner cases can partially be hidden due to
this idealized model. We believe finer granularity of the evaluation could uncover
clearer positive effect of our use of math in the process.

Besides searching for better evaluation strategies, our further research will
investigate learning-to-rank methods to pick up the most representative MTerms.
We will test this method with other features of structured data, such as syntactic
or dependency trees. It might be useful to further experiment with the ‘tokenization’ of math to smaller semantic elements, possibly better reflecting the specific notation used in different disciplines, to effectively imitate successful text processing techniques (such as the normalization of word forms) with mathematical content.

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