SCIENTIFIC DATA

RELISH-DB a large expert-curated database for benchmarking biomedical literature search.

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Abstract

Document recommendation systems for searching relevant literature have mostly relied on methods developed a decade ago. This is largely due to the lack of a large offline gold-standard benchmark of relevant documents that cover a variety of research fields such that newly developed literature search techniques can be compared, improved and translated into practice. To overcome this bottleneck, we have established the **RE**levant **LI**terature **S**earc**H** consortium of more than 1,500 scientists in 84 countries, who have collectively annotated the relevance of over 180,000 PubMed articles with regard to their respective seed (input) article/s. The majority of annotations were contributed by highly experienced, original authors of the seed articles. The collected data covers 76% of all unique PubMed MESH descriptors. No systematic biases were observed across different experience levels, research fields, or even time spent on annotations. More importantly, the same document pairs annotated by different researchers are highly consistent with each other. We further show that three representative baseline methods [Okapi Best Matching 25 (BM25), Term Frequency–Inverse Document Frequency (TF-IDF), and PubMed Related Articles (PMRA)] have similar overall performance. The database server located at `https://relishdb.ict.griffith.edu.au` is freely available for data downloading and blind testing of new methods.

Background & Summary

Drafting a research manuscript like this article requires a survey of relevant literature or related articles in the same sub-field. Traditionally, such a survey is conducted by a combination of searches based on selected keywords and

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[†] A full list of members appears in the Author Contributions

references in citations (the references cited by and to selected articles). This process often requires multiple attempts of different keyword combinations and examinations of numerous references cited. Often a mixed, long list of relevant and irrelevant articles has to be manually separated after further reading and yet not all important, relevant articles are necessarily included after this long, tedious process. The task of finding truly relevant articles becomes increasingly time consuming and challenging as the number of scientific articles published every year expands at a rapid pace. For example, the PubMed collection (`http://www.ncbi.nlm.nih.gov/pubmed`) for the last three years have seen a sustained annual growth rate of nearly 5%, from 25.2 million records in 2015 [7], 26.4 million records in 2016 [8] and now over 27.5 million in 2017 [9]. Finding the right keyword combinations is the key for ensuring the completeness and precision of the search.

One way to avoid keywords in search is to employ a seed-article. A seed-article can provide the title, the abstract, citations, and even its full text, containing significantly more information than a combination of a few pre-selected keywords. Such article-based relevance search, often referred as the research-paper recommender system, is an active area of research with more than 100 different approaches published since 1998 [3]. Examples of commonly-used methods are Okapi Best Matching 25 (BM25) [18, 19], Term Frequency–Inverse Document Frequency (TF-IDF) [29] and PubMed Related Articles (PMRA) [22]. These and other decade-old methods remain the backbone behind real world recommender systems such as PubMed, ReseachGate (`http://www.researchgate.net`), and CiteULike (`http://www.citeulike.org`). Numerous new methods developed are not yet translated into practice because it is not clear if new technologies have improved over traditional methods [3].

Improvements in paper recommender systems can be measured by *user studies*, *online evaluations* or *offline evaluations*. The problem with user studies and online evaluations is that large amount of active participation is required to infer any meaningful conclusions [3]. A large-scale user study would require costly recruitment and management of a large number of participants, whereas for online evaluations it is challenging to attract large numbers of active users to a deployed system except for a few systems with large user bases such as PubMed [13]. However, such information is often not made publicly available. Additionally, online evaluations collect implicit measures of satisfaction such as click-through-rates, however, non-clicked items are not necessarily an indicator of negative samples.

Offline evaluations, on the other hand, require a gold standard benchmark to compare and contrast the performances of different systems. Previous work has focused on building gold standards of query-to-document relevance in biomedical literature. Queries are generally defined as some topic comprised of a natural language statement, question, or set of keywords conveying a specific information need. Representative examples of existing gold standard query-to-document resources include the OSHUMED [14] collection, the TREC [32] Genomics track (the only biomedical focused track within TREC [15]), the BioASQ [31] competition and the bioCADDIE [6] dataset. While these datasets are suitable for benchmarking information retrieval with regards to the satisfaction of particular queries, they do not take into consideration the similarity between pairs of documents as a whole. Efforts have been made to re-purpose these types of datasets to the document-to-document level, for example, adaptation of the 2004/2005 TREC Genomics data [16, 17] has been employed by previous studies [22, 5, 33] for evaluation. However, two documents may be related to a certain topic but not necessarily to each other as complete units. Additionally, it has been concluded recently that 'there is unfortunately no existing dataset that meets the need for a machine-learning–based retrieval system for PubMed, and it is not possible to manually curate a large-scale relevance data set' [13].

Here, we have made the impossible possible by establishing the RELISH (**RE**levant **LI**terature **S**earc**H**) consortium of 1,500+ scientists from 84 countries around the world. The consortium has annotated over 180,000 document-document pairs indexed by PubMed, nearly 400 times larger than the only other human annotated data collection we could find with just 460 annotations by 90 authors [23]. The analysis of data collected indicates the diversity and the consistency of annotations among different levels of research experience as well as its usefulness in benchmarking different document-document comparison methods.

Methods

The overall procedure for establishing the RELISH database is as follows. First, we established the article-based PubMed search engine (APSE) at `https://pubmed.ict.griffith.edu.au` for recommending potentially relevant articles (*candidate-articles*) for an input article (*seed-article*) given by or assigned to a user. The APSE allows users to assess and annotate recommended candidate articles regarding their degree of relevance to the respective seed-article and facilitating submission of these annotations. Then, we established the RELISH consortium of scientific authors (*participants*) and invited them to the APSE to evaluate 60 candidate articles for one or more seed-articles that they have authored or are interested in. To ensure annotation quality each participant was encouraged to evaluate seed-articles of which they have authored. Finally, submitted annotations from participants were compiled and organized into the RELISH database. A participant *contribution* is defined as the submission of annotations for all 60 candidate-articles with respect to a seed-article. The remainder of this section gives specific details regarding database construction including APSE's corpus data and candidate article recommendation methods, participant recruitment and annotation procedures, and performance evaluation metrics.

APSE: Document corpus

The seed-article corpus used by the APSE server is the biomedical literature from PubMed. The corpus database was constructed with the 2017 baseline downloaded from NLM's public FTP server, followed by incremental synchronization with daily update releases. Only articles with both title and abstract metadata available were included in the corpus. As of July 3rd 2018, this collection contains 18,345,070 articles of which participants could select seed-articles from.

The candidate-article corpus, from which the APSE server generates recommendations presented to participants, is a subset of the seed-article corpus. This subset includes only recent articles that were published within the last decade. The primary justification for this is to increase participant motivation with potential discovery of recent work within their field, considering the decline of participation willingness according to publication age as speculated by [34]. As of July 3rd 2018, this candidate-article subset contains 8,730,584 articles.

All raw article texts were pre-processed into usable indexing elements (tokens) by the following pipeline. We first applied Lucene's *UAX29URLEmailTokenizer* which follows Unicode Text Segmentation rules [10] to divide the text (whilst also tagging detected URLs or email addresses). Next, possessives (trailing 's) were removed from each token, and any single character, numeric, URL or email tokens were removed. Stop-word tokens were filtered according to a list of 132 official MEDLINE stop-words retrieved from [2]. Finally, tokens were stemmed to their root form using Lucene's *PorterStemFilter*.

APSE: Recommendation system

The APSE recommendation system is built on three baseline methods: PubMed Related Articles (PMRA) [22], BM25 [18, 19] and TF-IDF [29]. PMRA is the technique used by the 'Similar Articles' function on the official PubMed site, here we used the Entrez E-utilities [21] ELink to retrieve related articles for given seed-articles. BM25 is a representative probabilistic based relevance technique and was implemented here by Lucene's *BM25Similarity* class using default parameters of $k1 = 1.2$ and $b = 0.75$. TF-IDF is a representative vector space model technique which was implemented here by Lucene's *ClassicSimilarity* class.

To generate the recommended list, we took the individual result lists of the above three search methods and combined them into a unified list. Each method's list of candidate articles was sorted by descending score. We set a maximum of 60 articles per seed-article as to include at least the top-20 highest scoring non-redundant candidate articles per method. That is, any overlapping articles (the same recommendation generated by multiple methods) are only added once to the final recommendation list upon first encounter, with the next best scoring unseen candidate taken from other methods; for evaluation purposes however, original lists from each method are used. This unified list of recommendations is not presented in the order of predicted similarity. Instead, prior to presentation to the user, it was shuffled into a random order to reduce the possibility of systematic bias in annotation.

RELISH: Participant recruitment

To achieve the goal of a large dataset facilitating future deep learning-based method development, we established the RELISH consortium of biomedical researchers who have annotated potentially related studies for one or more seed-articles that they have authored or are interested in. To maximize the quality and efficiency of annotation, we encouraged participants to use articles that they have authored as the seed-articles. All participants contributed voluntarily, the only incentive was that the order of the consortium member list would reflect the number of contributions made by participants. Only submissions with complete annotations for all 60 recommended candidate-articles per seed-article were accepted.

Our recruitment strategy involved two major phases: the first was internal referrals, personal invitations, social media posts, and a correspondence letter [4]; the second was to directly contact authors of papers published in 2018. For this secondary phase, we built a contact list of the corresponding authors with 2018 papers indexed in PubMed Central [28], and created a personalized email with the top-3 candidate-articles (the highest scoring non-redundant document from each method) for their article along with an invitation to join our consortium. The majority of received contributions resulted from this phase.

RELISH: Annotation procedure

An overview of the annotation procedure is shown in Figure 1. Each participant is asked to annotate the degree of relevance (*relevant*, *somewhat-relevant* or *irrelevant*) between a seed-article and a recommended candidate-article. We gave the following definitions for the degrees of relevance as a guide for label assignment:

- **Relevant**: the article is topically relevant to the input article, it is within the same specific sub-field of research; i.e. an article that you would be interested to read further, or could have been cited within the work.
- **Somewhat-relevant**: the article is missing some key topical details from the input article, it is within the broader area of research but does not specifically fit into the sub-field; i.e. unlikely to be included as a citation within the work.
- **Irrelevant**: the article is unrelated to the input article and obviously does not fit inside the specific sub-field of research.

Although definitions of 'relevance' are subjective, we aim to make the choice as simple as possible by utilizing this three-point degree of document pair 'closeness', as opposed to higher degrees of freedom like the five or ten point scales. Additionally, this three-point scale is more suited to the application of binary classification (a two-point 'positive' or 'negative' scale). Prior to annotation submission, contributors were asked to provide their level of experience from the following options: PhD student, number of years post-PhD (less than 5 years, between 5 to 10 years, or more than 10 years) and other (unspecified).

Evaluation metrics

The expert-annotated document pairs provide the opportunity to evaluate the performance of the three baseline methods for the first time. To simplify the evaluation, we limit ourselves to two-state classification in which, unless stated otherwise, *relevant* seed-candidate article pairs are assigned to the 'positive' class, while *somewhat-relevant* and *irrelevant* article pairs are assigned to the 'negative' class. Using this classification, we assess method performances with both binary classification and information retrieval metrics.

For binary classification metrics, we employed Matthews Correlation Coefficient (MCC) and Area Under the [receiver operating characteristic] Curve (AUC). MCC measures two-class classification quality [25], determined by a threshold parameter of the similarity score that separates positives from negatives. Here we report the maximum value. It is a balanced measure even when the distribution of positive and negative class instances is unbalanced [1], where a value of 1 represents perfect prediction and a value of 0 represents random prediction. AUC is determined by a receiver operating characteristic curve, a plot of sensitivity as a function of specificity at varying threshold parameter values. The area under this ROC curve yields the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative instance [12], where a value of 1 represents perfect prediction and a value of 0.5 represents random prediction.

Metrics for information retrieval include precision of top-N ranked results (P@N) and the Mean Reciprocal Rank (MRR) which considers the position of the first 'positive' item in a result-list. Averaging the RR over a sample of queries Q gives the mean reciprocal rank (MRR). P@N and MRR metrics emphasize high-ranked 'positive' class results, on the grounds that the first page of results is critical for users of web-scale search technology.

Infrastructure

The database search infrastructure is powered by Elasticsearch[1] (using Apache Lucene[2]). The web interface was designed with React[3], our web services were built with Apache[4] and Python[5] and our data is organized using MongoDB[6]

Data Records

A complete dump of collected annotation data as at July 3rd 2018 was deposited to a figshare repository available at `https://figshare.com`. All data records were stripped of personally identifiable information, and then converted to JSON

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[1] `https://github.com/elastic/elasticsearch`

[2] `https://github.com/apache/lucene-solr`

[3] `https://github.com/facebook/react`

[4] `https://github.com/apache/httpd`

[5] `https://github.com/channelcat/sanic`

[6] `https://github.com/mongodb/mongo`

format [20]. Record fields include PubMedID of the seed-article (*id*), annotator experience level (*experience*), and annotator response (*response*) containing the lists of candidate-article PubMedIDs corresponding to the assigned degree of relevance (i.e. one of *relevant*, *partial* (somewhat-relevant) or *irrelevant*).

Technical Validation

Annotations were contributed by a diverse group of highly experienced original authors

All annotations completed up to July 27th, 2018 have been consolidated into the initial revision of RELISH-DB. Table 1 shows simple statistics of the RELISH database content according to research experience level of participants. Annotations were received from a total of 1,643 unique scientists around the world, of which 1,570 are registered participants (affiliated consortium members) and 73 contributed anonymously. Figure 2 shows contributors to this project coming from diverse geological locations including 84 unique countries with the largest clusters located in Europe (586), North America (356), China (265) and Oceania (161). Altogether, the participants have annotated 3,017 seed-articles or 181,020 (3,017×60) labelled document pairs. The average number of submissions per participant is 1.9 (all anonymous submissions were considered as individuals), the majority of participants (77%) submitted annotations for just one seed-article, 11% for two, 3% for three, and 1% for four and five, respectively. A few dedicated participants annotated more than 50 seed-articles. The majority of contributions (63%) were made by highly experienced researchers with 5 or more years experience after their PhD degree. More significantly, the majority of seed-articles (91%) were evaluated by one of the original authors according to name matches. These statistics suggest high quality annotations within the RELISH database.

Annotations cover diverse research areas

Figure 3 shows a word cloud distribution of MESH descriptor frequency for all annotated documents, normalized by baseline frequencies in all PubMed documents. There appears to be no obviously strong bias towards any specific field. The diversity of annotated content is also illustrated by a 76% coverage of all unique MESH descriptors in the official PubMed library collection by the documents in the RELISH database (seed + candidate articles). Such a diversity in research fields is important for benchmarking literature search tools applicable for all research fields within biomedical research.

Partial relevance is the most popular annotation

The distribution of the three possible relevance labels (relevant, somewhat-relevant and irrelevant) across all contributions per seed-article is shown in Figure 4. The peaks for relevant and somewhat-relevant annotations is at 8

(102 articles, 3.4%) and 21 (111 articles, 3.7%), respectively, indicating that many articles fall into the grey area of partial relevance. For irrelevant annotation, the distribution peaks at 0: 9.7% of all seed-articles have no irrelevant candidate-articles annotated. The overall dominance of relevant and somewhat-relevant annotations suggests the reasonable performance of three methods for locating documents with at least somewhat relevance to the seed-articles.

Consistency of annotations according to method performance

Our definition of relevance, somewhat relevance and irrelevance is subject to different interpretations by different individuals. In order for a document recommendation system to work well, some commonality among these subjective opinions have to exist. To examine if such commonality exists, we compare the performance of the three baseline methods on annotations made by scientists of different experience levels, annotations of same articles by different individuals, and annotations across different research fields and different amounts of time spent. To make this comparison, we removed 44 seed-articles that PMRA provided less than 20 candidate article recommendations for and 186 responses that did not have any candidate articles marked as positive (relevant) or negative (somewhat relevant or irrelevant). In addition, we set aside 154 duplicate annotations of the same seed-article by different participants (named 'D154'). This leads to a total of 2,633 seed-articles (the ALL set, 'ALL2633'). From this set we derive a 'NR' (non-redundant) set, comprised of a single seed-article from each unique participant to avoid potential bias against specific annotators. In this dataset, for participants with multiple seed-article contributions, only one seed article was selected at random. This 'NR' set has 1,514 seed-articles ('NR1514'). Here we define somewhat relevance and irrelevance as negative samples to challenge three baseline methods and measure the performance according to two-state classification.

Consistency between all and non-redundant sets

Table 2 compares performance of the three baseline methods between the all set ('ALL2633') and the non-redundant ('NR1514') sets. The table shows essentially comparable performance between the three methods, with TF-IDF having the slightest edge. Moreover, overall the trend is shared between the 'W2633' and 'NR1514' sets, showing that the participants with multiple seed-article annotations have not biased the overall result. This is likely due to the majority of all unique participants submitting annotations for a single seed-article only. Another interesting observation is that PMRA produced the most candidate-articles marked as relevant (indicated by average precision @ 20), but seemed to have difficulty ranking them all towards the top of the result list. For MCC and AUC, TF-IDF is statistically significantly above PMRA (p-values $<$ .05 for 'W2633' and $<$ .004 for 'NR1514') and for MRR and P@5, both TF-IDF and BM25 are statistically significantly better than PMRA (p-values $<$ .005 for 'W2633' and $<$ .04 for 'NR1514').

Consistency among different experience levels

Figure 5 shows AUC given by PMRA, BM25 and TF-IDF across annotators in different levels of research experience. There is clearly no statistically significant difference between AUCs of the three methods and among different levels of experience (except for the 'PhD[$>$10y]' and 'other' groups, where TF-IDF is statistically significantly above PMRA). There is also no statistical difference between the methods for both P@5 and P@10 (pvalue $>$ .08). It should be noted that although the overall average is nearly identical among different experience levels, the fluctuations around the average (~0.2) is quite significant. This large fluctuation, however, may not be caused by the subjective opinions of individuals. In fact, if we examine the results from three dedicated contributors who annotated a large number of article pairs, there is a similar level of fluctuations in AUC values between different seed articles within a single contributor (Table 3). However, as method performance is so close overall, there appears to be some noise regarding the preferred methods with other annotator groups. Precision-based metrics for A1 demonstrate fluctuation of 'difficulty' with regard to the number of 'positive' annotations per seed-article. With P@20 of around 0.1, means that each method on average was trying to rank 2 articles higher than 18 other irrelevant articles which must have large content-based similarity of some form to be initially detected by these baseline methods. In contrast, A2 and A3 are relatively easier, especially considering the MRR value close to 1, meaning that on average the top-1 result was actually relevant. This suggests that the fluctuation may be due to the small size of samples (20) per seed-article per method for calculating the various measures.

Consistency among different research fields

Here we assessed performance consistency across very different research topic areas. Figure 6 shows method AUC across the largest clusters of documents sharing a MeSH qualifier. The eight topic areas include: Mice ('D051379'), Molecular Models ('D008958'), Protein Binding ('D011485'), Algorithms ('D000465'), Mutation ('D009154'), Protein Conformation ('D011487'), Computational Biology ('D019295') and Biological Models ('D008954'). It is apparent that there is no significant performance deviation between these topics.

Consistency among different annotators for the same document pairs

A more direct assessment of consistency is to examine the same document pairs annotated by different contributors, the 'D154' set. These contributions cover a total 74 unique articles. However, 32 articles were removed due to duplicate annotation submissions from a single participant (i.e. the same participant contributed annotations more than once for the same seed-article). There were also 2 articles which were annotated by three participants. In total, 40 unique articles remain in this consistency set (a total of 80 / 154 contributions, each article here is annotated by exactly two unique participants). We measured the agreement by using two state classifications and calculating the Jaccard index, which is defined as the intersection size of same positive annotations plus the intersection size of same negative annotations divided by the union size of all annotations. The distribution of the Jaccard index can be seen in Figure 7, where the overall trend appears to indicate strong consistency, with only 3 cases below 50% overlap. The average annotation consistency is 75%. In one of the low agreement cases, we contacted the original contributors and found that one annotator defines relevance by ‘AND’ (satisfaction of all topic keywords) whereas the other by ‘OR’ (as long as it contains one essential topic keyword). Nevertheless, there is consistency amongst the majority of dual-annotated document pairs.

Consistency between time spent for annotations

An additional consistency aspect we explored was the amount of time a participant spent making their annotations. This time was estimated between the time of loading the first page of results and time of submission. As this time was estimated, and is likely to contain a small degree of error due to noise in the logs, for this evaluation we restricted the time spent to between 2 and 120 minutes. Figure 8 demonstrates method performance as a function of time spent on annotations for the ‘NR’ set. Shown in the figure is bin size (blue bars, left y-axis) and method performance (blue, orange and green lines for PMRA, BM25 and TF-IDF respectively, right y-axis). As the majority of annotations were submitted within 17 minutes (75%), to equalize bin size as much as possible, bin intervals had to be varied across x-axis (not uniform sized). We can see that there is no obvious correlation between time spent on annotations and resulting method performance, indicating that there is no systematic bias underlying time spent for annotations.

Consistency among thresholds for two-state classification

Defining positives from negatives requires a threshold for the similarity score calculated by PMRA, BM25, or TF-IDF. An ideal method should have the same threshold for different seed articles regardless the size of abstracts/titles and the fields of studies so that only relevant articles are recommended, rather than a fixed number of recommendations. We analyze the distribution of method score thresholds in Figure 9. Raw method scores were first normalized using min-max method and then divided into 50 equal sized bins. It can be seen that all of the method threshold distributions are relatively centralized around their respective peaks, however, it is clear that PMRA compared to other methods has the most stable cutoff values with a standard deviation of .06, compared to .08 and .09 by BM25 and TF-IDF respectively, suggesting the possibility to set a unified relevance cutoff.

Difference between three methods

Figure 10 examines true relevant articles uniquely contributed by each method (PMRA, BM25 or TFIDF in the top panel) and the overlaps among them. It can be seen that in most cases that PMRA produces the largest proportion of relevant articles (avg. 17%) not given by BM25 and TFIDF (additionally highlighted by the average P@20 for PMRA) whereas BM25 has the lowest contribution of unique relevant recommendations (avg. 8%). Meanwhile, the overlap among them is low with the highest between BM25 and TFIDF at 32% on average. Thus, it is clear that no method can provide a complete coverage of relevant articles. Relatively few recommendations shared by all three methods indicate the possibility of a well-performing hybrid method which aggregates results from multiple methods.

Usage Notes

To make RELISH collections useful for future method developers, we have established a data server at `https://relishdb.ict.griffith.edu.au`. This data server has three modules for data annotation, data retrieval, and method testing, respectively.

- **Data Annotation:** Data annotation functions in exactly the same way as the APSE server. As shown in Figure 1, users can search for relevant publications to any article of interest, with the option to voluntarily annotate article relevance for the generated list of recommendations. Any new submissions will be automatically saved for inclusion in the next version of the database.

- **Data Retrieval:** We have made available several pre-built datasets for download after excluding a random collection set aside for blind prediction. They include the All and NR sets at different experience levels. In addition, several large single-annotator data sets are also made available separately. We also have an option to allow users to generate a dataset according various pre-defined parameters (dataset size, experience level, single-seed-article or multiple-seed-article annotators, and cut offs for number of relevant or irrelevant recommended articles per seed-article). As shown in Figure 11, pre-compiled datasets can be inspected by starting at (1), alternatively, user-defined datasets may be generated by starting at (2). After creating a new dataset or clicking on an existing one the dataset view page will be displayed , shown in stage (3). Here, the dataset details including size, number of positive and negative pairs, and any custom generation parameters that were set will be given. For each dataset, we make available the respective subsets of article metadata, annotation data, and an example result file in the format the automatic evaluation will accept, shown in stage (4). The metadata includes the PubMed ID, title and abstract for each article involved in the dataset. Since we are using publicly licensed PubMed metadata, we allow for direct download of this metadata in JSON format [20]. Relevance data is provided in TREC relevance format [26]. Method developers can divide downloaded datasets into training and independent test sets according to their own specific needs.

- **Method Testing:** To facilitate comparison and avoid over-training, we set aside a blind test set for critical assessment of method performance. This selection of 400 randomly selected NR seed-articles have their annotation data withheld from the rest of the database (although the data was included for presented evaluations within this manuscript). The dataset has two variants (BT1 having usual parameter of articles marked as partially relevant being counted as 'negative', and BT2 counting these partially relevant articles as 'positive'). Baseline method performances are shown in Table 4. Overall, this trend is consistent with what is observed for the complete dataset. We envision that method developers can download pre-built or user-defined datasets for training and independent tests. Then they download BT1 or BT2 to provide additional tests by submitting the result file in TREC result format [27] as shown in Stage (5) of Figure 7. Evaluations will be automatically performed and a list of recorded evaluations for the dataset will be shown in stage (6). After uploading a result file for a new evaluation or clicking on an existing evaluation in the list will display evaluation results; firstly a summary of metrics over the dataset as a whole is given by stage (7) and secondly the metrics are broken down into a per seed-article query basis for inspection in stage (8).

Discussion

This work represents a community-wide effort to establish a database of document relevance that is suitable for machine-learning. More than 1,500 scientists around the world participated in the RELISH consortium and annotated the relevance for over 180,000 document-document pairs of which covers diverse research fields characterized by 76% of all PubMed MESH descriptors without clear dominance (Figure 3). These annotations are of high quality as more than 90% of the article pairs were annotated by original authors and 63% by scientists with 5 or more years of research experience after their PhD degree. While the majority annotated a single seed article, a few dedicated researchers annotated more than 50 seed articles, and some independently annotated the same seed articles. Together, the resulting dataset provides the largest manually annotated benchmark for biomedical literature search.

Potentially subjective bias is one major concern for manual annotations of document relevance by such a diverse group of scientists. If such bias exists, one would expect that the performance of three baseline methods (PMRA, BM25 and TF-IDF) has certain systematic trends. We showed that the method performance is nearly the same across different experience levels (Figure 5), different research topic area (Figure 6), and different amount of time spent in annotation (Figure 8). Although the magnitude of the performance fluctuation is large between different annotators, the same magnitude of fluctuation is observed within the same annotator (Figure 5), suggesting that the source of fluctuation is likely due to the small size of samples (20 per seed-article for each method). More importantly, examining same document-document pairs annotated by different researchers indicates a high average consistency of 75% (Figure 7). Furthermore, high consistency in the dataset is also suggested from relatively narrow distribution of thresholds that were used to maximize the Matthews correlation coefficient for each seed-article (Figure 9). This indicates that the relevance can be defined across different experience levels or research fields. All of these indicate that while the subjective bias does exist, there is a consensus regarding what is relevant literature for the majority of researchers, despite difference in areas of research and experience levels.

High quality data collected by the RELISH consortium offers the unprecedented opportunity to compare three baseline techniques (PMRA, BM25, and TF-IDF). Somewhat surprisingly, all three methods have very similar performance with TF-IDF having a slight edge. This is somewhat different from earlier studies [24, 11, 30] where the classic TF-IDF is often considered as inferior than methods developed afterwards. Nevertheless, all three methods evaluated in this study perform only moderately well with an average AUC around 0.7 and MCC around 0.5. Moreover, different methods can capture different sets of relevant articles (Figure 10). This indicates significant room for improvement by future method development. To assist unbiased evaluation and avoid overtraining, we have made the RELISH database freely accessible to the academic community. Moreover, we set aside of 400 × 60 document-document pairs for blind prediction with automatic evaluation by our database server at `https://relishdb.ict.griffith.edu.au`.

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Author contributions

P.B. participated in design, carried out the study, and wrote the manuscript; RELISH consortium performed the annotations; Y.Z. conceived the study, participated in the initial design, assisted in data analysis, and wrote the manuscript; all authors read, contributed to the discussion, and approved the final manuscript.

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Epidemiology, Johns Hopkins Bloomberg School Of Public Health; 1505. Clinical Research And Evidence-Based Medicine Unit, Second Medical Department, Aristotle University Thessaloniki; 1506. Kfu-Riken Translational Genomics Unit, Riken; 1507. Dep. Of Systems Neuroscience, University Of Goettingen; 1508. Department Of Physiology And Pharmacology, Karolinska Institutet; 1509. Division Of Mental Health And Addiction, Institute Of Clinical Medicine, University Of Oslo; 122. Institute For Cancer Genetics And Informatics, Oslo University Hospital; 1510. Division Of Rehabilitation And Agein, University Of Nottingham; 1511. Surgery, Kansai Medical University; 1512. Research Services, Alpha-Altis; 1513. Uwa Dental School, University Of Western Australia; 1514. Genetics And Genomics, The Roslin Institute, University Of Edinburgh; 658. Institute Of Public Health - Section Of Hygiene, Catholic University Of The Sacred Heart, Rome, Italy; 1515. Nhmrc Clinical Trials Centre, University Of Sydney; 1516. Pharmacology, Universitat De Valènca; 1517. Internal Medicine, University Of New Mexico Health Sciences Center; 1518. Biomedical Engineering, University Of Bridgeport; 1519. Orthopaedics & Rehabilitation, University Of Florida; 1520. Focas Research Institute, Dublin Institute Of Technology; 1521. Department Of Medicine, University Of Oslo; 1522. Computational And Systems Biology, University Of Pittsburgh; 1523. Hellenic Cord Blood Bank, Biomedical Research Foundation Academy Of Athens; 1524. Caribbean Institute For Health Research, The University Of The West Indies; 1525. Child & Adolescent Psychiatry, Child Study Center At Hassenfeld Children'S Hospital Of New York At Nyu Langone; 1526. Department For Internal Medicine Ii, University Clinic Krems, Karl

Landsteiner University For Health Sciences; 1527. Institute Of Biophysics, Dezhou University; 1528. Department Of Cardiovascular Surgery, Maastricht University; 1529. Pain Center, , Daejeon St. Mary'S Hospital; 1530. Biotechnology, All India Institute Of Medical Sciences; 1531. Classics, Royal Holloway; 1532. Medicine, Ross University School Of Medicine; 1533. School Of Biological Sciences, University Of Nebraska-Lincoln; 1534. Structural And Molecular Biology, Ucl; 1535. Faculty Of Kinesiology, University Of Calgary; 1536. Ciet, University Of Costa Rica; 1537. Trauma & Orthopaedics, Wrightington Hospital; 1538. Pharmaceutical Chemistry, University Of Kwazulu Natal; 1539. Neuroscience, Carleton University; 1540. Ob-Gyn, New York University; 1541. Psychiatry, University Of Pennsylvania; 1542. Institute For Advanced Bioscience, Cnrs; 1543. Melbourne School Of Population And Global Health, University Of Melbourne; 1544. Epidemiology And Biostatistics, University Of Arizona; 1545. Anesthesiology, University Of Colorado Denver Anschutz Medical Campus; 1546. Department Of Pharmacology And Experimental Neuroscience, University Of Nebraska Medical Center; 1547. School Of Veterinary Sciences, Massey University; 1548. The Renal And Metabolic Division, Faculty Of Medicine & Health Sciences, The George Institute For Global Health, Macquarie University; 1549. Agriculture And Agri-Food Canada, Lacombe Research And Development Centre; 1550. Mechanical Engineering, University Of Birmingham; 1551. Edmond & Lily Safra Center For Brain Sciences, Hebrew University Of Jerusalem; 580. Institute For Glycomics, Griffith University; 1151. Ict, Griffith University

Competing financial interests

The author(s) declare no competing financial interests.

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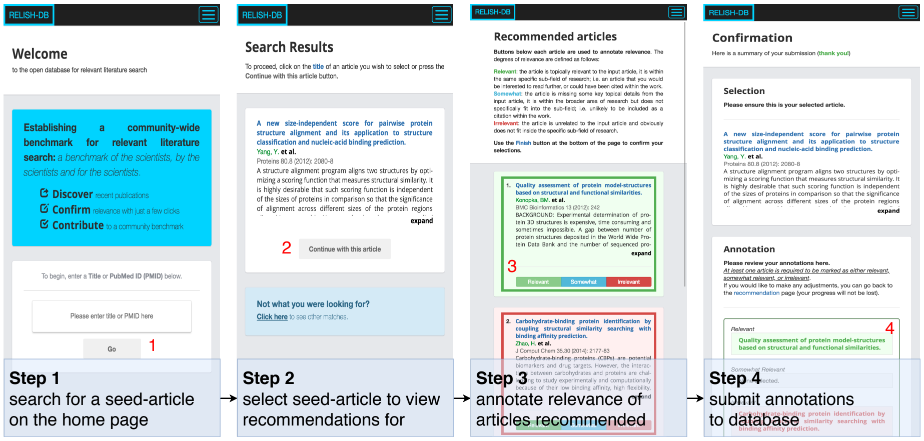


Welcome

to the open database for relevant literature search

Establishing a community-wide benchmark for relevant literature search: *a benchmark of the scientists, by the scientists and for the scientists.*

- **Discover** recent publications
- **Confirm** relevance with just a few clicks
- **Contribute** to a community benchmark

To begin, enter a **Title** or **PubMed ID (PMID)** below.

Step 1
search for a seed-article on the home page

Search Results

To proceed, click on the title of an article you wish to select or press the **Continue with this article** button.

A new size-independent score for pairwise protein structure alignment and its application to structure classification and nucleic-acid binding prediction.
Yang, Y. **et al.**
Proteins 80.8 (2012): 2080-8
A structure alignment program aligns two structures by optimizing a scoring function that measures structural similarity. It is highly desirable that such scoring function is independent of the sizes of proteins in comparison so that the significance of alignment across different sizes of the protein regions

Not what you were looking for?
Click here to see other matches.

Step 2
select seed-article to view recommendations for

Recommended articles

Buttons below each article are used to annotate relevance. The degrees of relevance are defined as follows:

Relevant: the article is topically relevant to the input article, it is within the same specific sub-field of research; i.e. an article that you would be interested to read further, or could have been cited within the work.
Somewhat: the article is missing some key topical details from the input article, it is within the broader area of research but does not specifically fit into the sub-field; i.e. unlikely to be included as a citation within the work.
Irrelevant: the article is unrelated to the input article and obviously does not fit inside the specific sub-field of research.

Use the Finish button at the bottom of the page to confirm your selections.

1. **Quality assessment of protein model-structures based on structural and functional similarities.**
Konopka, BM. **et al.**
BMC Bioinformatics 13 (2012): 242
BACKGROUND: Experimental determination of protein 3D structures is expensive, time consuming and sometimes impossible. A gap between number of protein structures deposited in the World Wide Protein Data Bank and the number of sequenced pro-

2. **Carbohydrate-binding protein identification by coupling structural similarity searching with binding affinity prediction.**
Zhao, H. **et al.**
J Comput Chem 35.30 (2014): 2177-83
Carbohydrate-binding proteins (CBPs) are potential biomarkers and drug targets. However, the interac-

Step 3
annotate relevance of articles recommended

Confirmation

Here is a summary of your submission (thank you!)

Selection

Please ensure this is your selected article.

A new size-independent score for pairwise protein structure alignment and its application to structure classification and nucleic-acid binding prediction.
Yang, Y. **et al.**
Proteins 80.8 (2012): 2080-8
A structure alignment program aligns two structures by optimizing a scoring function that measures structural similarity. It is highly desirable that such scoring function is independent of the sizes of proteins in comparison so that the significance of alignment across different sizes of the protein regions

Annotation

Please review your annotations here.
At least one article is required to be marked as either relevant, somewhat relevant, or irrelevant.
If you would like to make any adjustments, you can go back to the recommendation page (your progress will not be lost).

Relevant
Quality assessment of protein model-structures based on structural and functional similarities.

Somewhat Relevant

Step 4
submit annotations to database

Figure 1: An overview of the four stages comprising the annotation procedure. In step 1, the title or PubMed ID of a desired seed-article is searched; in step 2 a seed-article is selected; in step 3 the result-list is presented to participant for annotation; in step 4 all annotations are reviewed before being submitted to the database.

Figure 2: Distribution of participant geo-location, there are 1,570 registered participants from 84 unique countries, the majority of contributors are from Europe, North America, China and Australia.

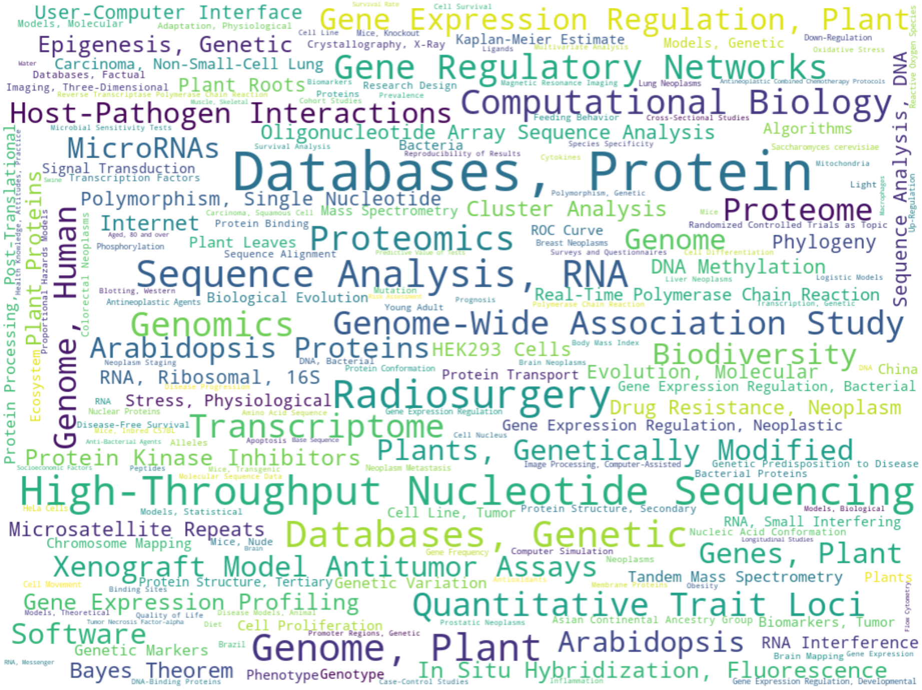


Figure 3: Word cloud of the 250 most frequent MESH qualifiers from all seed-articles normalized by frequencies in the whole PubMed library. In total, unique qualifiers present in the seed-article collection cover 76% of all unique MESH qualifiers.

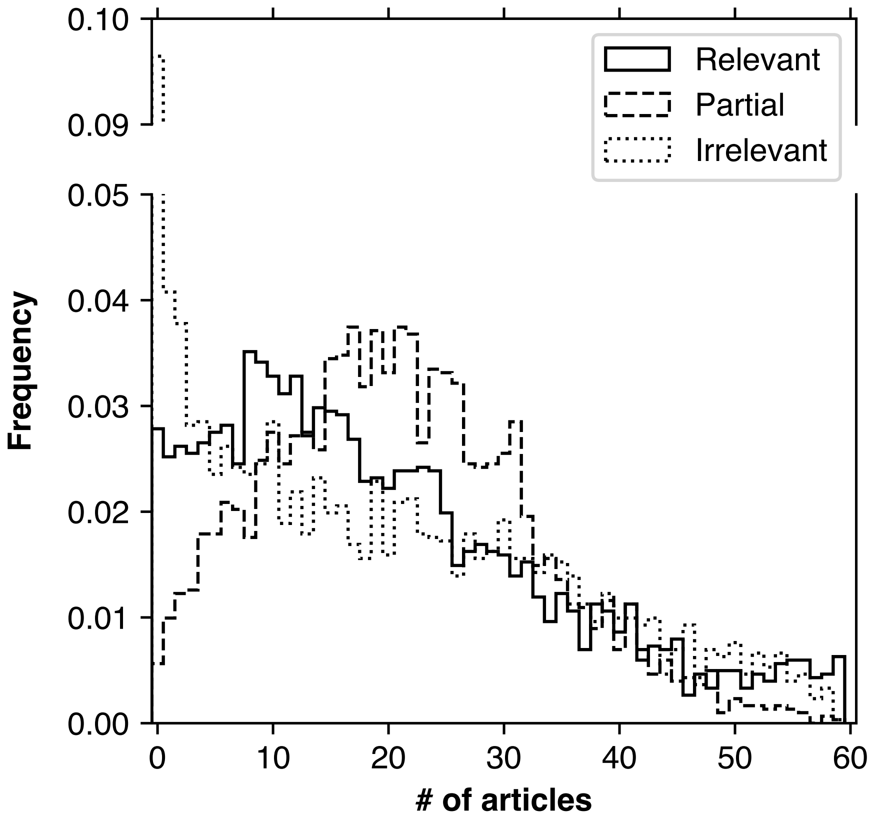


Figure 4: Frequency of seed-articles (y-axis) containing n annotated candidate-articles of respective labels (x-axis).

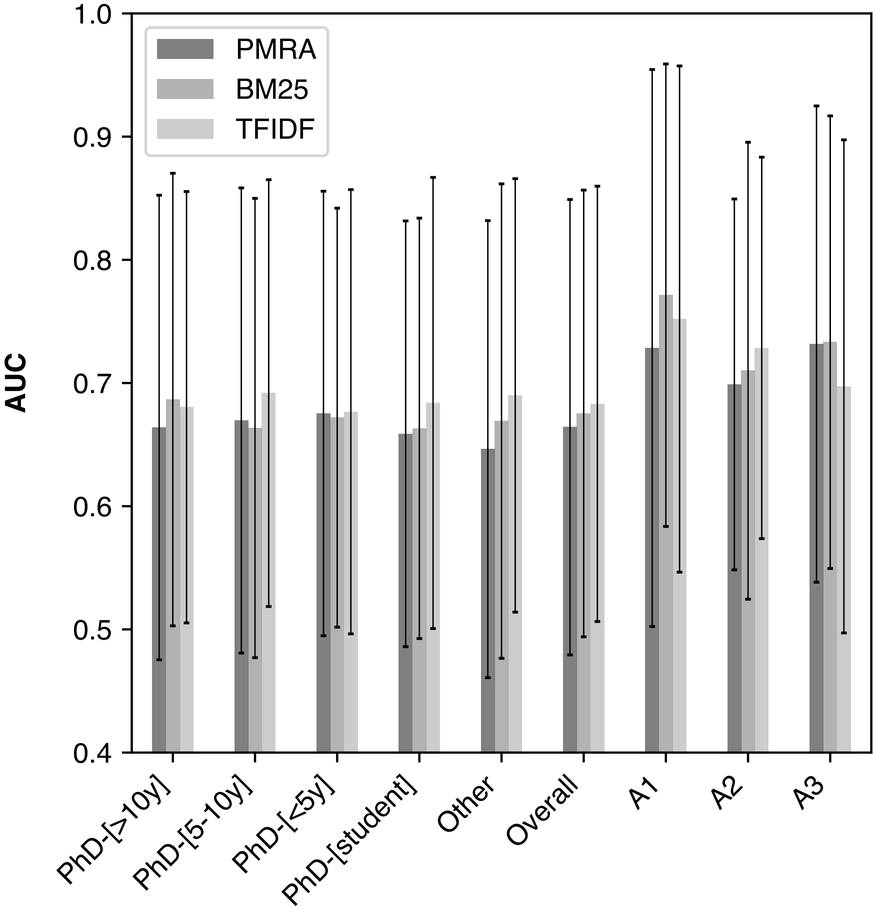


Figure 5: Method performance in terms of average Area Under the ROC Curve (AUC) for PMRA, BM25 and TF-IDF on the 'NR' set across annotators with experience levels and within three individual annotators (A1, A2 and A3).

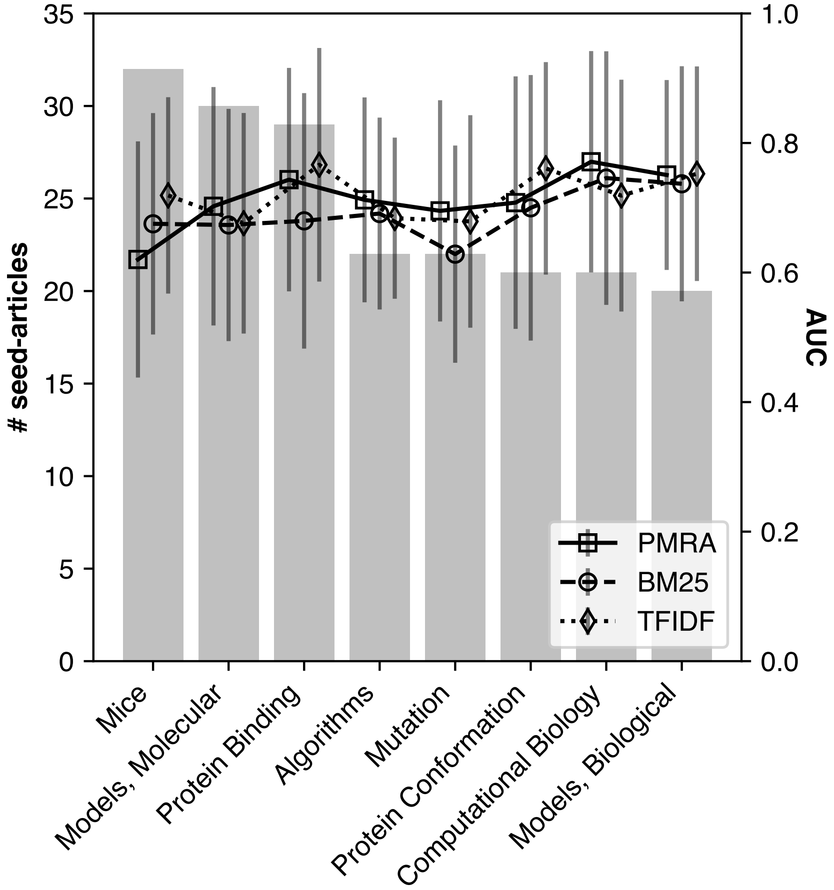


Figure 6: Method performance in terms of AUC across 8 different research areas; Mice ('D051379'), Molecular Models ('D008958'), Protein Binding ('D011485'), Algorithms ('D000465'), Mutation ('D009154'), Protein Conformation ('D011487'), Computational Biology ('D019295') and Biological Models ('D008954'). Bars correspond to number of seed-articles in the topic area, whereas lines indicate method performance according to AUC values.

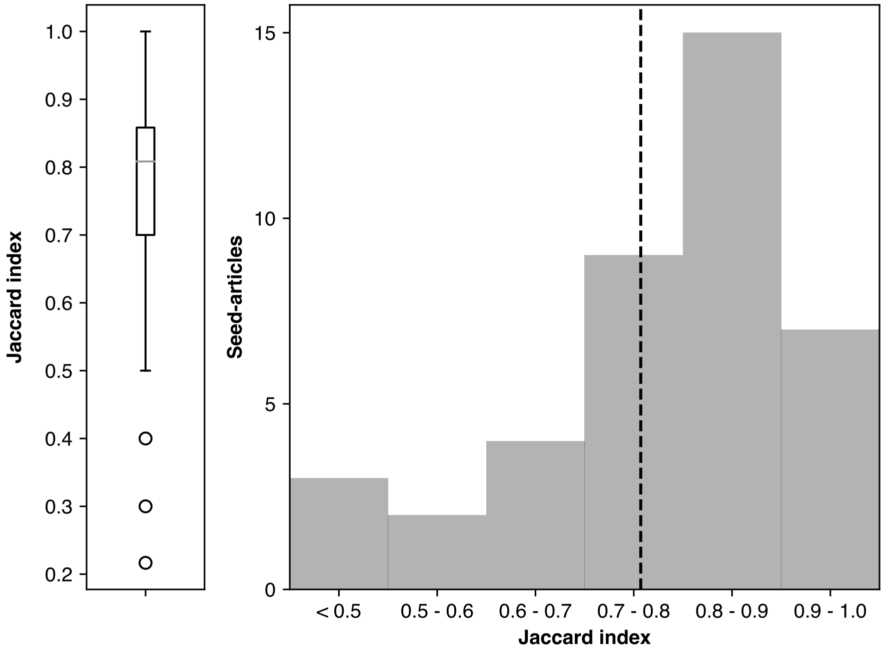


Figure 7: Agreement between different annotators for the same seed-article using Jaccard Index shown as average (left panel) and distribution (right panel).

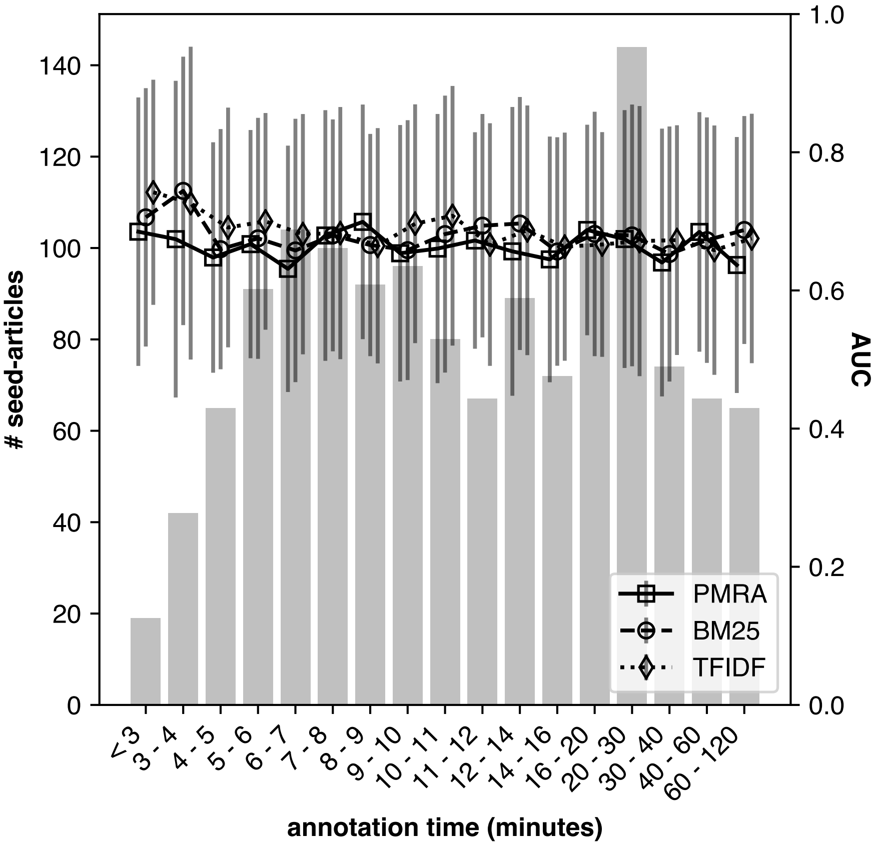


Figure 8: Method performance as a function of annotation time spent for the 'NR' evaluation set; X-axes are binned time-spent in minutes; vertical bars corresponding to left Y-axes are number of seed-articles per bin; lines corresponding to right Y-axes show average AUC per bin for PMRA, BM25 and TF-IDF methods respectively.

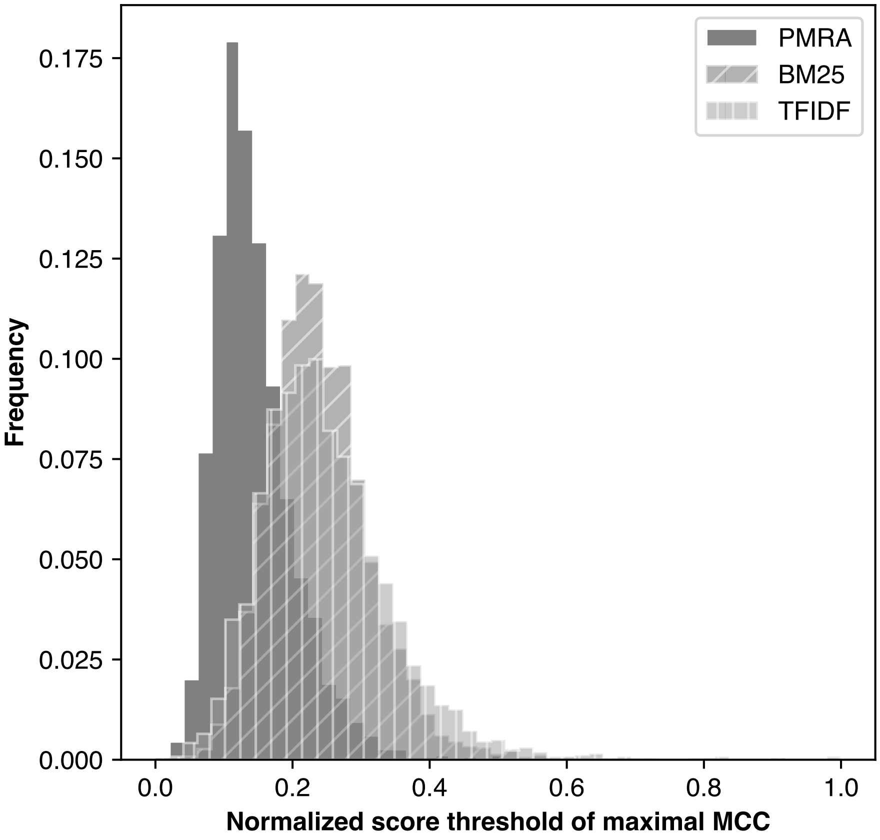


Figure 9: Distribution of method scores yielding highest MCC value per seed-article.

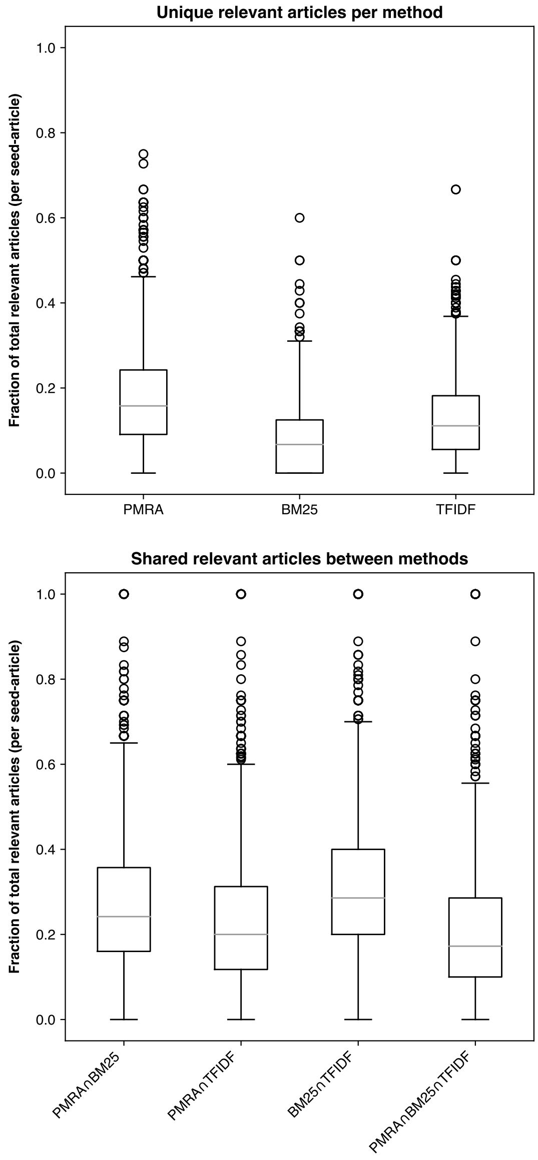
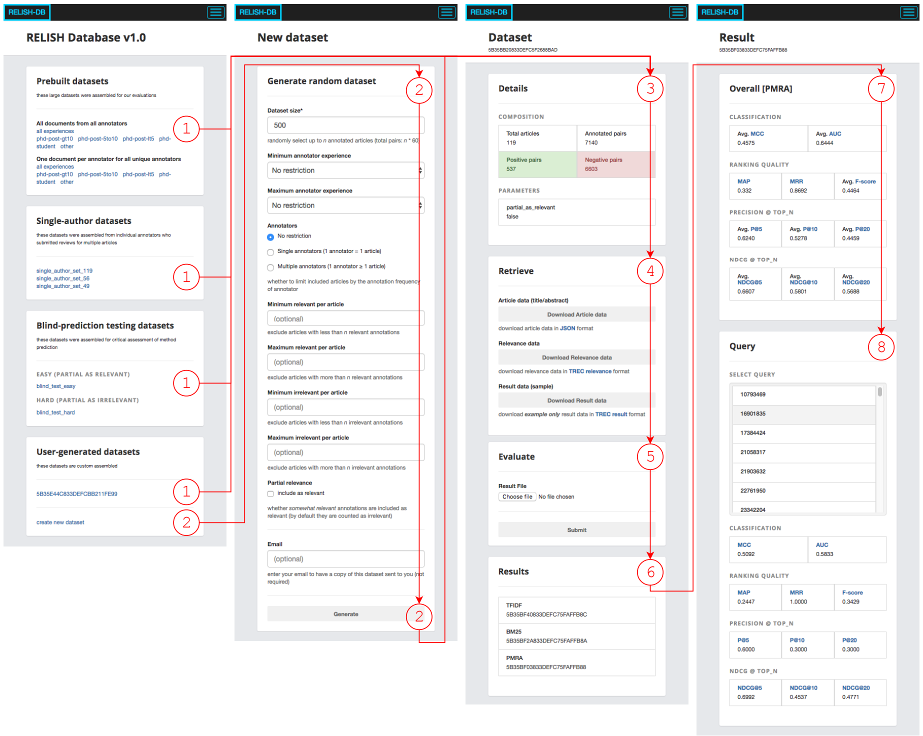


Figure 10: Consistency and difference among three methods; upper - unique relevant recommendations given by each method, lower - overlap of relevant recommendations between methods.



RELISH Database v1.0

Prebuilt datasets

these large datasets were assembled for our evaluations

All documents from all annotators
all experiences
phd-post-gt10 phd-post-5to10 phd-post-lt5 phd-student other

One document per annotator for all unique annotators
all experiences
phd-post-gt10 phd-post-5to10 phd-post-lt5 phd-student other

Single-author datasets

these datasets were assembled from individual annotators who submitted reviews for multiple articles

single_author_set_119
single_author_set_56
single_author_set_49

Blind-prediction testing datasets

these datasets were assembled for critical assessment of method prediction

EASY (PARTIAL AS RELEVANT)
blind_test_easy
HARD (PARTIAL AS IRRELEVANT)
blind_test_hard

User-generated datasets

these datasets are custom assembled

5B35E44C833DEFCBB211FE99

create new dataset

New dataset

Generate random dataset

Dataset size*: 500
randomly select up to *n* annotated articles (total pairs: *n* * 60)

Minimum annotator experience: No restriction

Maximum annotator experience: No restriction

Annotators
● No restriction
○ Single annotators (1 annotator = 1 article)
○ Multiple annotators (1 annotator ≥ 1 article)
whether to limit included articles by the annotation frequency of annotator

Minimum relevant per article: (optional)
exclude articles with less than *n* relevant annotations

Maximum relevant per article: (optional)
exclude articles with more than *n* relevant annotations

Minimum irrelevant per article: (optional)
exclude articles with less than *n* irrelevant annotations

Maximum irrelevant per article: (optional)
exclude articles with more than *n* irrelevant annotations

Partial relevance
☐ include as relevant
whether *somewhat relevant* annotations are included as relevant (by default they are counted as irrelevant)

Email: (optional)
enter your email to have a copy of this dataset sent to you (not required)

Dataset
5B35BB20833DEFC5F2688BAD

Details

COMPOSITION

Total articles 119	Annotated pairs 7140
Positive pairs 537	Negative pairs 6603

PARAMETERS

partial_as_relevant
false

Retrieve

Article data (title/abstract)
download article data in **JSON** format

Relevance data
download relevance data in **TREC relevance** format

Result data (sample)
download *example only* result data in **TREC result** format

Evaluate

Result File: No file chosen

Results

TFIDF
5B35BF40833DEFC75FAFFB8C

BM25
5B35BF2A833DEFC75FAFFB8A

PMRA
5B35BF03833DEFC75FAFFB88

Result
5B35BF03833DEFC75FAFFB88

Overall [PMRA]

CLASSIFICATION

Avg. MCC	Avg. AUC
0.4575	0.6444

RANKING QUALITY

MAP	MRR	Avg. F-score
0.332	0.8692	0.4464

PRECISION @ TOP_N

Avg. P@5	Avg. P@10	Avg. P@20
0.6240	0.5278	0.4459

NDCG @ TOP_N

Avg. NDCG@5	Avg. NDCG@10	Avg. NDCG@20
0.6607	0.5801	0.5688

Query

SELECT QUERY

10793469
16901835
17384424
21058317
21903632
22761950
23342204

CLASSIFICATION

MCC	AUC
0.5092	0.5833

RANKING QUALITY

MAP	MRR	F-score
0.2447	1.0000	0.3429

PRECISION @ TOP_N

P@5	P@10	P@20
0.6000	0.3000	0.3000

NDCG @ TOP_N

NDCG@5	NDCG@10	NDCG@20
0.6992	0.4537	0.4771

Figure 11: An overview of the database retrieval and evaluation process: (1) use existing datasets - both pre-built and user-generated; (2) create custom datasets - allows for user-defined dataset construction by tuning dataset generation parameters; (3) dataset details - shows the size, number of positive and negative pairs, and any custom parameters used to generate; (4) dataset article data - allows user download of (a) raw article metadata (id, title and abstract) (b) annotation data and (c) sample result file for evaluation function; (5) result file upload - allows input of result files for automatic performance assessment; (6) uploaded evaluations - results of uploaded result file evaluations for the respective dataset will be presented here; (7) overall evaluation view - provides a performance summary of the dataset as a whole; (8) detailed evaluation view - performance details are broken down on a per-query basis

Table 1: Distribution of database content by participant experience level. *Registered* and *Anonymous* columns show number of participants at respective experience levels. *Contributions* is the total number of seed-articles evaluated by participants at respective experience levels.

	Registered	Anonymous	Contributions
PhD-[>10y]	652 (41.5%)	34 (46.6%)	1,391 (46.1%)
PhD-[5-10y]	249 (15.9%)	7 (9.6%)	512 (17.0%)
PhD-[<5y]	283 (18.0%)	14 (19.2%)	538 (17.8%)
PhD-[student]	191 (12.2%)	11 (15.1%)	282 (9.3%)
Other	195 (12.4%)	7 (9.6%)	294 (9.7%)
Total	1,570	73	3,017

Note: contribution total includes both registered and anonymous submissions.

Table 2: Overall evaluation set performance results. 'All' includes all seed-articles from all participants. 'NR' includes only one seed-article from each participant.

		#	MCC	AUC	MRR	P@5	P@10	P@20
All	PMRA	2,633	0.494 ± 0.22	0.675 ± 0.18	0.850 ± 0.28	0.612 ± 0.30	0.534 ± 0.28	0.456 ± 0.26
	BM25		0.507 ± 0.22	0.683 ± 0.18	0.859 ± 0.28	0.616 ± 0.30	0.527 ± 0.28	0.448 ± 0.26
	TFIDF		0.507 ± 0.22	0.685 ± 0.18	0.874 ± 0.27	0.628 ± 0.30	0.534 ± 0.28	0.454 ± 0.26
NR	PMRA	1,514	0.481 ± 0.22	0.664 ± 0.18	0.862 ± 0.27	0.631 ± 0.29	0.552 ± 0.27	0.475 ± 0.26
	BM25		0.502 ± 0.21	0.675 ± 0.18	0.873 ± 0.26	0.629 ± 0.29	0.541 ± 0.27	0.461 ± 0.25
	TFIDF		0.504 ± 0.21	0.683 ± 0.18	0.886 ± 0.25	0.646 ± 0.29	0.550 ± 0.27	0.468 ± 0.26

Table 3: Method performance for the three largest single-annotator sets.

		#	MCC	AUC	MRR	P@5	P@10	P@20
A1	BM25	92	0.610 ± 0.25	0.771 ± 0.19	0.740 ± 0.34	0.335 ± 0.19	0.226 ± 0.13	0.150 ± 0.09
	PMRA		0.580 ± 0.26	0.728 ± 0.23	0.726 ± 0.35	0.313 ± 0.19	0.212 ± 0.11	0.149 ± 0.08
	TFIDF		0.601 ± 0.27	0.752 ± 0.21	0.735 ± 0.35	0.337 ± 0.23	0.220 ± 0.13	0.155 ± 0.09
A2	BM25	55	0.538 ± 0.23	0.710 ± 0.19	0.882 ± 0.24	0.611 ± 0.29	0.498 ± 0.29	0.408 ± 0.27
	PMRA		0.547 ± 0.17	0.699 ± 0.15	0.892 ± 0.24	0.553 ± 0.28	0.420 ± 0.24	0.342 ± 0.22
	TFIDF		0.564 ± 0.20	0.729 ± 0.15	0.900 ± 0.25	0.615 ± 0.30	0.480 ± 0.28	0.377 ± 0.26
A3	BM25	49	0.550 ± 0.25	0.733 ± 0.18	0.966 ± 0.14	0.780 ± 0.22	0.698 ± 0.26	0.627 ± 0.28
	PMRA		0.561 ± 0.25	0.732 ± 0.19	0.944 ± 0.17	0.788 ± 0.24	0.718 ± 0.24	0.614 ± 0.28
	TFIDF		0.504 ± 0.25	0.697 ± 0.20	0.922 ± 0.20	0.710 ± 0.26	0.659 ± 0.29	0.605 ± 0.31

Table 4: Performance for the blind test set of 400 randomly selected articles.

		MCC	AUC	MRR	P@5	P@10	P@20
BT1	PMRA	0.467	0.668	0.974	0.884	0.834	0.771
	BM25	0.468	0.669	0.973	0.878	0.817	0.747
	TFIDF	0.491	0.683	0.990	0.894	0.822	0.760
BT2	PMRA	0.460	0.645	0.875	0.617	0.529	0.446
	BM25	0.482	0.662	0.888	0.613	0.510	0.414
	TFIDF	0.493	0.667	0.903	0.631	0.520	0.431