

Results

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First session

The initial search query for the example topic was:

((model OR models OR modeling OR network OR networks) AND (dissemination OR transmission OR spread OR diffusion) AND (nosocomial OR hospital OR “long-term-care” OR “long term care” OR “longterm care” OR “long-term care” OR “healthcare associated”) AND (infection OR resistance OR resistant))

selecting only results between 2010 and 2020 (included). Results were collected from Pubmed, WOS, IEEE, EMBASE and SCOPUS, using the framework tools as described in the Methods and Supplemental Material S1.

The first search session returned a total of 27,600 records, specifically 12,719 (71.6% of the total) records from the EMBASE database, followed by 9,546 (53.8%) from Pubmed, 3,175 (17.9%) from SCOPUS, 2,100 (11.8%) from WOS, and 60 (0.34%) from IEEE (Table 1). There were various degrees of overlapping between sources, with 38.4% of records being present in more than one database, and EMBASE and IEEE being the databases with the higher uniqueness ratios. The final data set was composed of 17,755 unique records. The first 250 records (based on “simple query ordering”) were categorised manually. Of these 43 (17.2%) were labeled as positive, and 207 (82.8%) as negative.

The categorised records were used to train the Bayesian classification model used to label the remaining records. After seven classification and review (CR) iterations (three resulting in new positive matches and four extra replications to account for stochastic variability), a total of 101 positives matches were found, requiring manual review of 766 records (13.2% positivity rate).

It is noticeable how the number of records that required manual review decreased rapidly between iterations (Table 2), indicating that the engine was converging while the uncertainties were resolved.

This phenomenon is better illustrated in Fig. 1 of Supplemental Material S2. It shows the mixture distribution of the PPDs of the records, specifically for records that were manually reviewed, before and after the classification step: it can be seen how the distribution of uncertain records shrinks (i.e., it becomes concentrated in a shorter probability range) and shifts toward the negative zone as more positive matches are found and reviewed.

We extracted the 15 more relevant terms for the classification model, described as: Term (citation part): Inclusion Rate (Inclusion Stability) [linear Relative Risk, Statistic]:

Patient Transport (Keyword): 61.2 (3.77) [99.1, 21.3], Transfer (Abstract): 57 (3.93) [22.5, 15.4], Network (Title): 56.5 (2.91) [18, 14.2], Network & Patient (Abstract): 54.2 (4.66) [26.3, 15.2], Donker T (Author): 53.5 (4.56) [159, 16.5], Worker (Abstract): 50 (3.33) [0.421, -1.21], Hospitals (Keyword): 49.8 (4.31) [27.8, 16.5], Movement (Abstract): 47.8 (2.7) [27.2, 15], Spread (Title): 46.6 (2.25) [16.2, 12.1], Facility (Abstract): 45 (2.22) [19.6, 14.8], Orange County (Keyword): 44.3 (3.19) [199, 17.2], Conduct (Abstract): 42.6 (3.7) [0.221, -2.57], Patient (Abstract): 42 (3.61) [27.6, 7.23], Perform (Abstract): 41.9 (2.38) [0.342, -2.55], Hospital (Title): 39 (1.95) [12.5, 12.5].

Table 1. Distribution of retrieved records by source and session. For each source, we reported the number of records, percentage over the session total (after removing duplicates), and the number of records specific for a source as absolute value and as percentage over the source total. All session shows records after joining and deduplication of the Session 1 and Session 2 data set.

Session	Source	Records	% over total	Source specific records	% over source total
Session1	Total	17,755			
	Embase	12,719	71.6%	6,683	52.5%
	Pubmed	9,546	53.8%	3,457	36.2%
	Scopus	3,175	17.9%	298	9.39%
	WOS	2,100	11.8%	473	22.5%
	IEEE	60	0.34%	29	48.3%
Session2	Total	82,579			
	Embase	48,396	58.6%	40,826	84.4%
	Pubmed	28,811	34.9%	18,021	62.5%
	Scopus	17,070	20.7%	4,908	28.8%
	WOS	12,956	15.7%	2,817	21.7%
	IEEE	61	0.074%	22	36.1%
All Sessions	Total	98,371			
	Embase	59,604	60.6%	46,942	78.8%
	Pubmed	37,278	37.9%	21,371	57.3%
	Scopus	19,353	19.7%	5,181	26.8%
	WOS	14,367	14.6%	3,175	22.1%
	IEEE	108	0.11%	48	44.4%

Table 2. Results of the automatic classification and manual review rounds. The cumulative numbers of positives and negative records and their sum (Total labelled) and percentage over total are shown for each iteration. Also, the number of changes after review and their description is reported. "Unlab." indicates unlabelled records marked for review. For each iteration, the number of features used by the engine is also reported. The first row reports the results of the initial manual labelling of records, which served as input for the automatic classification in Iteration 1. In Session 2, the engine uses the labels at the end of Session 1 to classify the newly added records.

Session	Iteration	Positives	Negatives	Total labelled (%)	Unlab. -> y	Unlab. -> n	Unlab. -> *	n -> y	Changes	N. features
Session1 (n = 17755)	Initial labelling	43	207	250 (1.41%)	43	207	0	0	250	2,289
	1	93	529	622 (3.5%)	50	322	0	0	372	2,289
	2	100	614	714 (4.02%)	6	86	0	1	93	3,750
	3	101	625	726 (4.09%)	1	11	0	0	12	3,834
	4	101	648	749 (4.22%)	0	23	0	0	23	3,856
	5	101	651	752 (4.24%)	0	3	0	0	3	3,856
	6	101	660	761 (4.29%)	0	9	0	0	9	3,856
	7	101	665	766 (4.31%)	0	5	0	0	5	3,856
	1	106	934	1040 (1.06%)	5	270	998	0	1,273	4,729
	2	107	1,123	1230 (1.25%)	1	189	0	0	190	4,729
Session2 (n = 98371)	3	107	1,176	1283 (1.3%)	0	53	0	0	53	4,733
	4	107	1,200	1307 (1.33%)	0	24	0	0	24	4,729
	5	107	1,209	1316 (1.34%)	0	9	0	0	9	4,729
	6	107	1,226	1333 (1.36%)	0	17	0	0	17	4,729

The “&” indicates nc-ngrams, i.e., terms strongly co-occurrent in the documents.

The engine was able to pick up the central concept of the research topic, i.e., “patient transport” or “transfer” through a “network” of “facility”ies that facilitates the “spread” of infections, and even one of the authors of this study (Donker T.) as well as the region of interest (“Orange County”) of another research group active on the topic of pathogen spreading over hospital networks. Some terms were considered highly relevant by

the BART models (e.g., “Worker” in the sixth position out of more than 3800 terms considered), although in a simple linear model, their effect would hardly be significant (statistic: -1.21 s.e.); these are terms that are only relevant in conjunction with other terms but not on their own, highlighting the extra predictive power achieved through the use of advanced, non-linear machine learning.

A more extensive set of terms is presented in Table 1 of Supplemental Material S2.

Second session

The results of the first classification session were used to create a second, data-driven query to perform a more extensive search to find records that may have been missed during the first search session. The resulting query was as follows:

((Donker T) NOT (bacterium isolate)) OR ((network patient) AND (resistant staphylococcus aureus) NOT (monte carlo) NOT isolation) OR (facility AND (network patient) AND regional NOT hospitals NOT increase NOT (patient transport) NOT (control infection use)) OR ((patient transport) NOT (Donker T) NOT worker) OR (hospitals AND (network patient) NOT (patient transport) NOT regional NOT clinical) OR (facility AND (network patient) NOT hospitals NOT (patient transport) NOT regional NOT prevention NOT medical) OR ((healthcare facility) NOT (Donker T) NOT worker NOT positive) OR (hospitals NOT (network patient) NOT medical NOT environmental NOT outcome NOT global) OR ((network patient) NOT facility NOT hospitals NOT (patient transport) NOT therapy NOT global)) AND ((antimicrobial resistance) OR (healthcare infection))

The final piece *AND ((antimicrobial resistance) OR (healthcare infection))* was added manually to define the search domain better since the algorithm was trained on documents that were all more or less related to these topics.

The generated query also provides a more nuanced understanding of the engine’s internal classification logic, and this is helpful to spot possible biases in the model.

The search was done with the same year filter and procedures used in the first session.

The new search produced 107,294 records (Table 1), of which 48,396 (58.6%) from the EMBASE, followed by 28,811 (34.9%) from Pubmed, 17,070 (20.7%) from SCOPUS, 12,956 (15.7%) from WOS, and 61 (0.074%) from IEEE; compared with the first session, the relative weight of EMBASE and Pubmed decreased, while the level of content specificity greatly increased, as it was for SCOPUS. After removal of duplicates, 82,579 unique records were obtained. The newly collected records were joined with those from the first session and duplicates were removed. We obtained 98,371 unique records, with just 1,963 shared records between searches, which equates to 2% of the total. The percentage of records shared by two or more sources dropped to 22%.

Six CR rounds were necessary to complete the second session classification, with just 6 new positive found after reviewing 568 extra records. The first CR iteration required the user to review a substantial number of records (1,273); however, just labelling 275 of them (the suggested 250 plus 25 already labelled for the framework hyperparameter tuning) was sufficient to reduce this number to just 190 in the subsequent round. An evaluation of the convergence (Supplemental Material S2, Fig. 1) showed that, in addition to the dynamics already observed in session 1 (shrinkage and negative shift), a second mode appeared in the mixture distribution of the records to be reviewed, centred in a highly positive zone. The interpretation is that as the number of negative training records increases, the engine becomes more and more sceptical and even asks to review some records labelled as positive in the initial training set generated during Session 1. This behaviour can reveal spot classification errors and inconsistencies. Considering both sessions, 1,333 records were manually reviewed and 107 (8.03%) confirmed positive matches were found.

Again, the evaluation of the inclusion rate of the terms showed that the engine is quite capable of internalising the concepts behind the research topic. A subsample of the relevant terms used by the model in the second session is reported in Table 2 of Supplemental Material S2.

Hyperparameter selection

As described in the methods, hyperparameters were selected by evaluating sensibility and efficiency through a grid search on a validation set of 1,200 manually labelled records. The analysis suggested that the following parameter combination performed best: an initial training set of 250 categorised records with 10x oversampling of positive matches, ten models in the ensemble, no bootstrapping and an uncertainty zone defined by the 98% predictive interval. This combination of parameters was associated with a sensitivity of 98.8% (81 / 82 positive matches found) and an efficiency of 61.5% (462 / 1200 records evaluated). The detailed results of the hyperparameter tuning analysis are reported in Table 3 of Supplemental Material S2. Fig. 2 in Supplemental Material S2 demonstrates that the positive record oversampling rate, the number of ensemble models and the size of the initial training set were the parameters that mainly impacted performance.

Performance evaluation

To evaluate the theoretical performance of the engine, a surrogate Bayesian logistic regression model was trained on the manually reviewed labels using only the lower boundary of the record PPDs as predictor (see the Methods for details). The surrogate model showed the high predictive power of the scores produced by the classification model (Bayesian R^2 : 98.1% [97.4%, 98.3%] for session 1 and 98.2% [97.6%, 98.3%] for session 2).

Fig. 2 presents the actual and predicted (from the surrogate model) cumulative number of positive matches, ordered by the initial simple ordering query: the median of surrogate models' cumulative predictive distributions matches the actual number of positive records found quite well. It is striking how many more records would have required manual evaluation to find the same number of positive matches without a classification algorithm, with some positive matches found close to the end of the heuristically ordered list of records.

Table 3 shows various performance indexes for both sessions, both descriptive (Total records, Reviewed records, Observed positive matches) and estimated through the surrogate model (Expected efficiency, Predicted positive matches, Expected sensitivity, R^2).

In session 1 we observe an expected total number of positives of 101 [101, 108] for an estimated sensitivity of 100% [93.5%, 100%] and efficiency of 95.6% [95.3%, 95.7%]. In session 2 we observed a drop in expected sensitivity, especially in the lower credibility boundary (97.3% [72.8%, 100%]): as the number of records increases, even a small probability of being a positive match can, in the worst-case scenario, lead to a relevant number of predicted positive matches (147 in this case). To ensure no obvious positive matches were missed, we evaluated 100 non-reviewed records with the highest median predicted probability and found no additional positive matches.

Table 3. Estimated performance summary. The table reports for each session, the number of reviewed records and the percentage over the total. Also, the posterior expected number of positive records, sensitivity and efficiency (as WSoR) are reported, with their 90% PrI truncated to the observed realisation in the dataset [trunc. PrI] (see. methods). Finally, the logistic model's median Bayesian R^2 [90% CrI] is reported. PrI: Predictive Intervals; CrI: Credibility Intervals.

Indicator	Session 1	Session 2
Total records	17,755	98,371
Reviewed records (% over total records)	766 (4.31%)	1,333 (1.36%)
Expected efficiency (over random) [trunc. 90% PrI]	95.6% [95.3%, 95.7%]	98.6% [98.1%, 98.6%]
Observed positive matches (% over total records)	101 (0.57%)	107 (0.11%)
Predicted positive matches [trunc. 90% PrI]	101 [101, 108]	110 [107, 147]
Expected sensitivity [trunc. 90% PrI]	100% [93.5%, 100%]	97.3% [72.8%, 100%]
Simple Model R^2 [90% CrI]	98.1% [97.4%, 98.3%]	98.2% [97.6%, 98.3%]

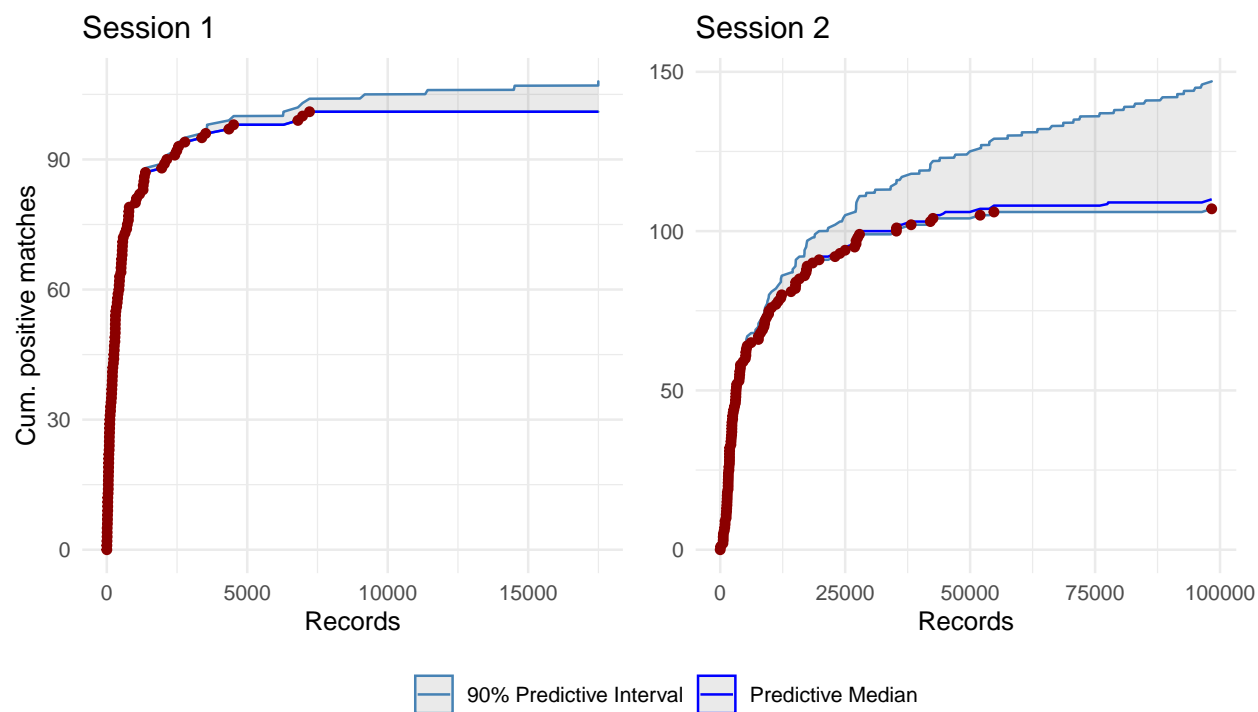


Figure 2. Observed cumulative number of positive matches (red dots) sorted by simple query ordering. The [trunc. 90% PrI] of the cumulative positive matches estimated by the Bayesian logistic model is shown as a shaded area delimited by the 95% quantile of the PrI and by the observed number of positive matches (light blue lines). A darker blue line represents the median of the PrI.