

# Predication-based Semantic Indexing: Permutations as a Means to Encode Predications in Semantic Space

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## Abstract

*Corpus-derived distributional models of semantic distance between terms have proved useful in a number of applications. For both theoretical and practical reasons, it is desirable to extend these models to encode discrete concepts and the ways in which they are related to one another. In this paper, we present a novel vector space model that encodes semantic predications derived from MEDLINE by the SemRep system into a compact spatial representation. The associations captured by this method are of a different and complementary nature to those derived by traditional vector space models, and the encoding of predication types presents new possibilities for knowledge discovery and information retrieval.*

## Introduction

The biomedical literature contains vast amounts of knowledge that could inform our understanding of human health and disease. Much of this literature is available as electronic text, presenting an opportunity for the development of automated methods to extract and encode knowledge in computer-interpretable form. Distributional models of language are able to extract meaningful estimates of the semantic relatedness between terms from unannotated free text. These models have proved useful in a variety of biomedical applications (for a review see (1)), and include recent variants that scale comfortably to large biomedical corpora such as the MEDLINE corpus of abstracts (2). However, the semantic relatedness estimated by most distributional models is of a general nature. These models do not encode the type of relationship that exists between terms, which limits their ability to support logical inference. Furthermore, while distributional models such as Latent Semantic Analysis (LSA) simulate human performance in many cognitive tasks (3), they do not represent the object-relation-object triplets (or propositions) that are considered to be the atomic unit of thought in cognitive theories of comprehension (4). In this paper we address these issues by defining Predication-based Semantic Indexing (PSI) a novel distributional model of language that encodes semantic predications derived from MEDLINE by the SemRep system (5) into a compact vector space representation. Associations captured by PSI complement those captured by existing models, and present new possibilities for knowledge discovery and information retrieval.

## Background

Many existing distributional models draw their estimates of semantic relatedness from co-occurrence statistics within a defined context such as a sliding window or an entire document (1). While recent models (reviewed in (6)) instead define as a context grammatical relationships produced by a parser, these models do not encode the nature of this grammatical relationship in a retrievable manner. The emergence of distributional models that incorporate word order (7), (8) has shown that it is possible to encode and retrieve additional information within a vector space. These models achieve this end by using either convolution products (7) or permutation of sparse random vectors (8) to transform vectors used to represent terms into new representations that are close-to-orthogonal to the original vectors. Consequently there is very little overlap in the information they carry, and additional information related to term position can be encoded. These transformations are reversible, to facilitate retrieval of this information.

PSI is based on Sahlgren and his colleagues' model which uses permutations as a means to encode word order information (8), which in turn is a variant of the Random Indexing (RI) approach to distributional semantics (9). This approach provides a simple and elegant solution to the problem of reversibly transforming term vectors using permutations of the sparse random vectors which form the basis of RI. Sahlgren *et al's* approach is derived from sliding-window (or term-term) RI, which bases its vector representations for terms on their co-occurrence with other terms in a sliding window moved through the text. While the sliding window approach is well-established in distributional semantics, established methods either use the full term-by-term space or reduce the dimensionality of this space using the computationally demanding Singular Value Decomposition (SVD). RI is able to achieve this dimension reduction step at a fraction of the computational cost of SVD by constructing semantic vectors for each term on-the-fly, without the need for a term-by-term matrix. Each term in the text corpus is assigned an elemental vector of dimensionality  $d$  (usually in the order of 1000), the dimension of a reduced-dimensional *semantic space* within which the semantic relatedness of terms will be measured. These elemental vectors are sparse: they contain mostly zeros, with in the order of 10 non-zero values of either +1 or -1. As there

are many possible permutations of these few non-zero values, elemental vectors tend to be close-to-orthogonal to one another: their relatedness as measured with the commonly used cosine metric tends towards zero. This approximates a full term-by-term matrix, but rather than assigning in orthogonal dimension to each term, RI assigns a close-to-orthogonal reduced-dimensional elemental vector. To encode additional information to do with word order, the elemental vector for a given term is permuted to produce a new vector, almost orthogonal to the vector from which it originated. Consider the low-dimensional approximations of elemental vectors below:

$V1: [10000100000-1000]$   $V2: [010000100000-100]$

These two vectors are orthogonal to one another: as there is no common non-zero dimension between them, their cosine (or normalized dot-product) will be zero.  $V2$  was derived from  $V1$  by rotating every value one position to the right, and conversely this transformation can be reversed by rotating every value in  $V2$  one position to the left. This simple procedure is used by Sahlgren *et al* to encode word-order information into a term-term based semantic space. The semantic vector for each term consists of the normalized linear sum of the permuted elemental vector for every term with which it co-occurs, with permutation encoding the relative position and direction of each term in the sliding window. The reversible nature of this transformation facilitates order-based retrieval. For example, a rotation one position to the right of all elements of the elemental vector for a term can be used to generate a vector with high similarity to terms occurring one space to the left of it. *Table 1* provides some examples of order-based retrieval in a permutation-based space created from the MEDLINE corpus of abstracts using the Semantic Vectors package, to which author TC is a contributor (10).

? cancer	streptococcus ?	? cough
.81:breast	.71:pyogenes	.89:whooping
.78:colorectal	.71:agalactiae	.48:nonproductive
.74:prostate	.69:pyogens	.47:hacking
.69:antiprostata	.65:milleri	.44:brassy
.67:antibreast	.62:acidominimus	.42:barking

**Table 1:** Order-based retrieval from MEDLINE. The “?” denotes the relative position of the target term.

In this paper, we adapt Sahlgren *et al*'s method of encoding word order information into a vector space to encode semantic predications produced by the SemRep system (5), (11). SemRep combines general linguistic processing, a shallow categorical parser and underspecified dependency grammar, with domain-specific knowledge resources: mappings from free text to the UMLS accomplished by the MetaMap software (12), the UMLS metathesaurus and semantic network (13) and the Specialist lexicon and lexical tools (14). SemRep

uses these techniques to extract semantic predications, from titles and abstracts in the MEDLINE database, as shown in this example drawn from (5). Given the excerpt “... *anti-inflammatory drugs that have clinical efficacy in the management of asthma,...*”, SemRep extracts the following semantic predication between UMLS concepts:

“Anti-Inflammatory Agents TREATS Asthma”

We present in this paper a description of the theoretical and methodological basis of PSI, and include examples of the sorts of information the model encodes and retrieves discussed in context of possible applications.

## Methods

We have derived a PSI space from a database of semantic predications extracted by SemRep from MEDLINE citations dated between 2003 and September 9<sup>th</sup> 2008. 13,562,350 predications were extracted from 2,634,406 citations by SemRep. Of these, predications involving negation (such as “DOES NOT TREAT”) are excluded, leaving 13,380,712 predications which are encoded into the PSI space. We encode this predication information using permutation-based RI. Rather than assigning elemental vectors to each term as in Sahlgren *et al*'s model, we assign sparse elemental vectors ( $d=500$ ) to each UMLS concept contained in the predications database. We then assign a unique number to each of the included predication types (such as “TREATS”). We create semantic vectors ( $d=500$ ) for each UMLS concept in the database, and every time a given UMLS concept occurs in a predication, we add to its semantic vector the elemental vector of the other concept in the predication. This elemental vector is permuted according to the type of the predication. For example, in the predication “Anti-Inflammatory Agents TREATS Asthma” we would add to the semantic vector for Anti-Inflammatory Agents but rotate every element in this 39 (the number assigned to the predicate “TREATS”) steps to the left. Conversely, we would add to the semantic vector for Asthma the index vector for Anti-Inflammatory Agents rotated 39 steps to the right. In this way we are able to encode the type of predication that exists between these concepts.

We also construct a general distributional model of the UMLS concepts in the database of predications using the Reflective Random Indexing (RRI) model (15), by creating document vectors for each unique PubMed ID in the database. Document vectors are created based on the terms contained in these citations: elemental vectors are assigned to each term, and document vectors are constructed as the normalized linear sum of the elemental vector for each term they contain. Rather than using raw term frequency, we employ the log-entropy weighting scheme, shown to enhance document representations in several applications (3). A vector for each concept is constructed as the frequency-weighted normalized linear sum of the vector for each document it occurs in.

PSI requires a modification of the conventional nearest neighbor approach, as we are interested in the strongest association between concepts across all predications. In the modified semantic network used by SemRep (16), there are 40 permitted predications between concepts when negations (e.g. exercise DOES NOT TREAT hiv) are excluded. Semantic distance in PSI is measured by extracting all permutations of a concept, and comparing the second concept to these to find the predication with the strongest association. For elemental vectors, we employ a sparse representation used in our previous work (2) which represents the dimension and sign of each of the 20 non-zero values. This allows for rapid generation of all possible permutations by augmenting the value that represents the index of each non-zero value. To speed up this process in the EpiphaNet example (Figure 1), we extract the 500 nearest neighbors to a cue concept from the general distributional space (this should subsume the predication-based space: every concept in a predication must co-occur in a citation with the other concept concerned). We then perform predication-based nearest-neighbor search on these neighbors only.

## Results and Discussion

### Predication-based retrieval

In a manner analogous to the order-based retrieval illustrated previously, it is possible to perform predication-based retrieval using permutations to determine which UMLS concept the model has encoded with strong association to another concept in a particular predication relationship. Table II illustrates predication-based retrieval. For example, the query “? TREATS Asthma” retrieves concepts for asthma treatments (sb-240563 is also known as Mepolizumab, and has recently been shown to reduce exacerbations in asthma (17)).

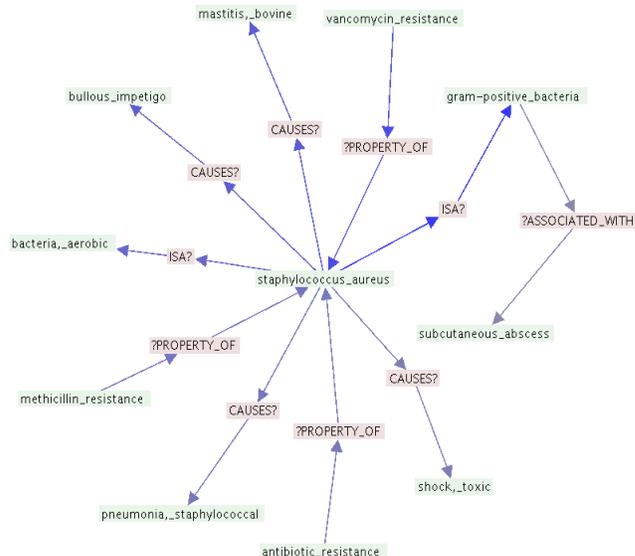
? TREATS Asthma	Metronidazole TREATS ?
1: cetirizine-pseudoephedrine	.57: chronic intestinal amebiasis
1: norisodrine	.36 : urogenital trichomonas nos
1: alvesco	0.35: erythema annulare centrifugum
1: salmeterol+fluticasone propionate	0.33: vaginalis
1: sb-240563	0.27: endocervicitis, unspecified

**Table II:** Predication-based retrieval with cosine associations between query and target concepts.

Interestingly, the top ranked results are not necessarily the concepts that occur most frequently in this predication relationship – rather, these results reflect the extent to which this relationship defines a particular concept, as the model represents concepts in terms of the predications in which they occur in an extensional

manner. Concepts occurring exclusively in a particular predication with another concept are likely to rank highly in predication-based retrieval. As this is not ideal for many purposes, our future work will explore variants of PSI that select for frequency rather than exclusivity.

### Predication-based Nearest Neighbor Search



**Figure 1:** EpiphaNet for “staphylococcus aureus”

It is possible to rapidly characterize a particular concept for exploratory purposes by first finding the  $k$  nearest neighbors in a general associative space, and searching amongst these for the best predications using PSI. Figure 1 illustrates the nearest predication-based neighbors of the concept “staphylococcus aureus” which we have extracted and visualized with the EpiphaNet software we have developed for this purpose. EpiphaNet is based on the Prefuse visualization library (18) and as in our previous work (2) uses Pathfinder network scaling (19) to reveal the most significant associative links within a network of near neighbors. By reversing the encoding process used in PSI, we are able to retrieve both the type and direction of the predication relationship linking these concepts. This measure of semantic distance is different in nature to those used in prior distributional models. Rather than conflating many types of association into a single metric, this estimate is based on the strongest typed association between these concepts across all predication-based relationship. Similarly to the way in which existing distributional models extract compact vector-based term representations from large corpora, the PSI model produces a compact representation for all UMLS concepts in the 8.8GB database of semantic predications. The set of semantic vectors used for the PSI space used to generate Figure 1 occupies 300MB only, and stored elemental vectors occupy a fraction of this space due to the sparse representation employed. To further assess the extent to which predications are accurately encoded and retrieved, we extract at random 1000 concepts, and retrieve their 20 nearest predication-

based neighbors. We consider neighbors with a cosine association above a threshold of the mean cue-to-neighbor association for these 1000 terms as “retrieved”. Using the database of predications extracted by SemRep as a gold standard, we calculate the following metrics:

- o Precision =  $\text{retrieved and accurate} / \text{all retrieved}$
- o Recall =  $\text{predications retrieved} / \text{minimum}(20, up)$

where  $up$  denotes the number of unique predications for cue term in the database. Results are shown in *Table III*.

Dimensionality	500	1000	1500
Mean Precision	0.957	0.977	0.997
Mean Recall	0.603	0.643	0.658
Threshold cosine	0.320	0.279	0.265

**Table III:** Results for 1000 randomly selected terms.

The model performs better for cue concepts with fewer unique predications: recall when only concepts with 20 or less unique predications are considered is 0.74, 0.8 and 0.8 at 500, 1000 and 1500 dimensions respectively, with precision at 0.95 and above. This suggests that vectors for concepts involved in many predication relationships acquire a spurious similarity to other vectors due to partial overlap between permuted elemental vectors. We anticipate this overlap would reduce as dimensionality increases. In practice we find that concepts such as “patient” that are involved in many unique predications tend to be uninformative. It is also possible to eliminate spurious neighbors by only considering terms that occur in a document with the cue term as retrieval candidates.

### Implicit Encoding of Semantic Type

As illustrated by the results of the cosine-based nearestneighbor search in *Table IV*, the PSI space to some extent captures the semantic class of UMLS concepts. The semantic vector for the disease “asthma” is similar to that for other diseases (and in this case, symptoms), just as “amitryptiline” retrieves other antidepressants through nearest neighbor search. This finding generalizes to a degree: amongst the ten-nearest neighbors of 1000 randomly selected terms, an average of 37% share a UMLS semantic type with the cue term. This is considerably higher than the result of approximately 4.5% obtained when the same evaluation is performed using either RI (9) or RRI (15) (all spaces at  $d=500$ ), and varies across semantic types, with several semantic classes such as “plant” exhibiting in excess of 80% agreement between cue and neighbor. This is to be expected, as the extraction of predications by SemRep is constrained by the UMLS semantic type of the subject and object. However, further analysis of the interplay between assigned UMLS class and predication-based distributional similarity may be a useful way to reveal inconsistencies in the assignment of semantic class and/or the assignment of predications by SemRep.

asthma	amitryptiline
.98: sickle cell anemia	.82: imipramine
.99 : heart septal defects, atrial	.78: nortriptyline
.99: chronic childhood arthritis	.76: desipramine
.98: diarrhea	.75: clomipramine
.98: constipation	.65: amoxapine

**Table IV:** Nearest-neighbor searches in PSI-space.

### Modeling Analogy

We find it is possible to model analogy within the PSI space by finding the predication that most strongly associates two terms and applying the rotation that corresponds to this predication to a third. While this work is presently at an early stage of development, it has produced some interesting results so far (*Table V*).

Example	Cue	Retrieved
Tuberculosis is to Isoniazid as.....	Depressive disorder is to..	Lexapro
Tuberculosis is to Lung X-ray as...	Depressive disorder is to..	Psychiatric Interview and Evaluation

**Table V:** Analogical Reasoning in PSI-space

### Application to Information Retrieval

Similarly to the way in which distributional models extract compact vector-based term representations from large corpora, the PSI model produces a compact representation of the predication relations captured by SemRep. The knowledge encoded in the PSI model could be used for information retrieval in several ways. One possibility would be to represent documents in terms of the predications contained therein, and allow users to search for documents containing concepts in a specific predication relationship with a search concept. We anticipate that once customized for this purpose, PSI will retrieve documents providing answers to clinical questions such as “what treats Tuberculosis” or “what causes Bullous Impetigo”. Another possibility would be the use of the approach taken in *Figure 1* to categorize documents according to the way in which they are related to a particular search concept. In our future work we will evaluate these approaches on standard test collections.

### Application to Literature-based Knowledge Discovery

In our recent work (2),(20),(15) we have used general distributional models to identify potential discoveries by identifying pairs of concepts that are relatively close in the space but do not co-occur in any of the documents in the database used to generate the models. Although this method has proven to be effective in identifying interesting indirect connections, the interesting ones tend to occur along with others of little interest. In general, additional constraints are needed to narrow the possibilities. The predications resulting from the methods presented here offer a promising means to limit the indirect connections by selecting those with appropriate

predication relationships. For example, when looking for new treatments for a disorder, concepts that serve as treatments should be given priority over concepts in other predications. With these methods, general word space similarity can be elaborated into the greater specificity found in semantic network models (21).

### Limitations and Future Work

This paper presents the theoretical and methodological basis for PSI, a novel distributional model that encodes predications produced by SemRep, and provides some illustrative examples and possible applications. Further analysis is needed to determine the model parameters that optimize performance in each of these tasks. In our future work we will explore applications of PSI to informatics problems, including information retrieval, knowledge discovery and biomedical question answering.

### Conclusion

PSI is a novel distributional model that encodes predications produced by the SemRep system, providing a more specific measure of semantic similarity between concepts than is provided by existing distributional models, as well as the ability to retrieve the type of predication that most strongly associates two concepts. From a theoretical perspective, this is desirable as the unit of analysis in cognitive models is considered to be an object-relation-object triplet, not an individual term. From a practical point of view, the additional information encoded by PSI is likely to be of benefit for information retrieval and knowledge discovery purposes. In our future work we will evaluate the application of PSI to these and other informatics problems.

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