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Introduction

Large amounts of biomedical data available to us today from various sources make it at least impractical and in many cases impossible to analyze by hand even if confined within a specific problem. On the other hand most of these data are stored in a natural language form which makes it hard to process automatically. Fortunately a vast experience gained in the field of natural language processing (NLP) can be utilized to automate this process. We developed an advanced parser for biomedical texts that should simplify both data retrieval and analysis.

We considered the following problems:

- 1. parsing of informative multiword phrases
- 2. parsing and detection of chemical names written in different notations - trivial notation and IUPAC and SMILES-like
- 3. assigning word embeddings for parsed words and phrases
- 4. analyzing complex syntactic dependencies between them

Methods

To improve parsing quality we decided to learn to extract informative n-grams (e.g. instead of ['amino', 'acid', ...] we want to get ['amino_acid', ...]) to account for existence of multiword biomedical terms.

To better identify informative n-grams and give a numerical estimate of their validity two main approaches were used.

First one relies on finding the most important edges in word collocation network for analyzed text. Word collocation networks are weighted directed graphs with each vertex corresponding to a word in the text and edge weights equal to the bigram frequency in the document. The most important edges are found by calculating centrality measures of network (degree, closeness, betweenness, etc.) or with the PageRank algorithm [Lahiri et al.]. This process can be applied to analyze documents separately or to generate a custom dictionary of ngrams from a large corpus of texts.

Second approach uses term frequency-inverse document frequency (TF-IDF) statistic. It rewards frequent terms inside a document but punishes words that are frequent in the whole corpus which helps to filter out the words that are just commonly used in a language.



 D_{variatio}



Collocation graph based on the abstract of [Harris et al, Stimulation of bone formation in vivo by phosphate supplementation. Calcif Tissue Res. 1976 Nov 24;22(1): 85-98.]. Stop-words were removed. Arrows skipped for convenience even though the graph is directed. Size of the node is proportional to its PageRank score.

Results

PageRank	Gaussian KL(bigram, token)	Gaussian KL(token, bigram)	Variationa
breast_cancer	ang_iii	citron_kinase	coli_isolate
cancer_cells	citron_kinase	biliary_complications	liver_cance
gene_expression	biliary_complications	vte_prophylaxis	hpv_dna
cell_lines	vte_prophylaxis	serum_calcium	model_gro
tumor_cells	new_drugs	dsrna_binding	molecular_
stem_cells	status_epilepticus	acute_ethanol	cardiac_fib
prostate_cancer	tuberculosis_isolates	hand_hygiene	early_disea
gastric_cancer	mrsa_strains	status_epilepticus	reported_c
cell_cycle	serum_calcium	ang_iii	genetic_stu
patients_treated	acute_ethanol	synthesized_compounds	meningoco
TF-IDF	Gaussian KL(bigram, token)	Gaussian KL(token, bigram)	Variationa
gene_expression	beta_sheet	beneficial_effects	related_pro
wild_type	disease_ad		
	_	results_mean	combinatio
present_study	beneficial_effects	results_mean self_renewal	significant
present_study cell_lines			
cell_lines	beneficial_effects	self_renewal	significant_
	beneficial_effects self_renewal	self_renewal remains_unclear	significant_ viral_rna
cell_lines amino_acid	beneficial_effects self_renewal old_woman	self_renewal remains_unclear efficacy_safety	significant_ viral_rna study_perfe
cell_lines amino_acid results_suggest breast_cancer	beneficial_effects self_renewal old_woman insulin_sensitivity	self_renewal remains_unclear efficacy_safety studies_performed	significant_ viral_rna study_perfe rat_model
cell_lines amino_acid results_suggest breast_cancer long_term	beneficial_effects self_renewal old_woman insulin_sensitivity et_al	self_renewal remains_unclear efficacy_safety studies_performed beta_sheet	significant_ viral_rna study_perfo rat_model tissue_spe
cell_lines amino_acid results_suggest	beneficial_effects self_renewal old_woman insulin_sensitivity et_al false_positive	self_renewal remains_unclear efficacy_safety studies_performed beta_sheet negative_bacteria	significant_ viral_rna study_perfo rat_model tissue_spec terminal_re

Kullback-Leibler Divergence

In the context of machine learning, $D_{KL}(P||Q)$ is often called the information gain achieved if P is used instead of Q.

$$D_{ ext{KL}}(P\|Q) = \sum_i P(i) \, \log rac{P(i)}{Q(i)}.$$

$$\sum_{a} (f \| g) = \sum_{a} \pi_{a} \log \frac{\sum_{a'} \pi_{a'} e^{-D(f_{a} \| f_{a'})}}{\sum_{b} \omega_{b} e^{-D(f_{a} \| g_{b})}}$$

KL-divergence method allows us to determine which sets of words are better to replace with an ngram as we can calculate the informativeness of ngram













References

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- 1. John R. Hershey and Peder A. Olsen, *Approximating the* 2. Luke Vilnis and Andrew McCallum, Word Representations via 3. Moz, Gaussian Word Embeddings, <u>https://github.com/</u>

