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Contrastive Clustering of medical reports to characterise Adverse Drug Reactions

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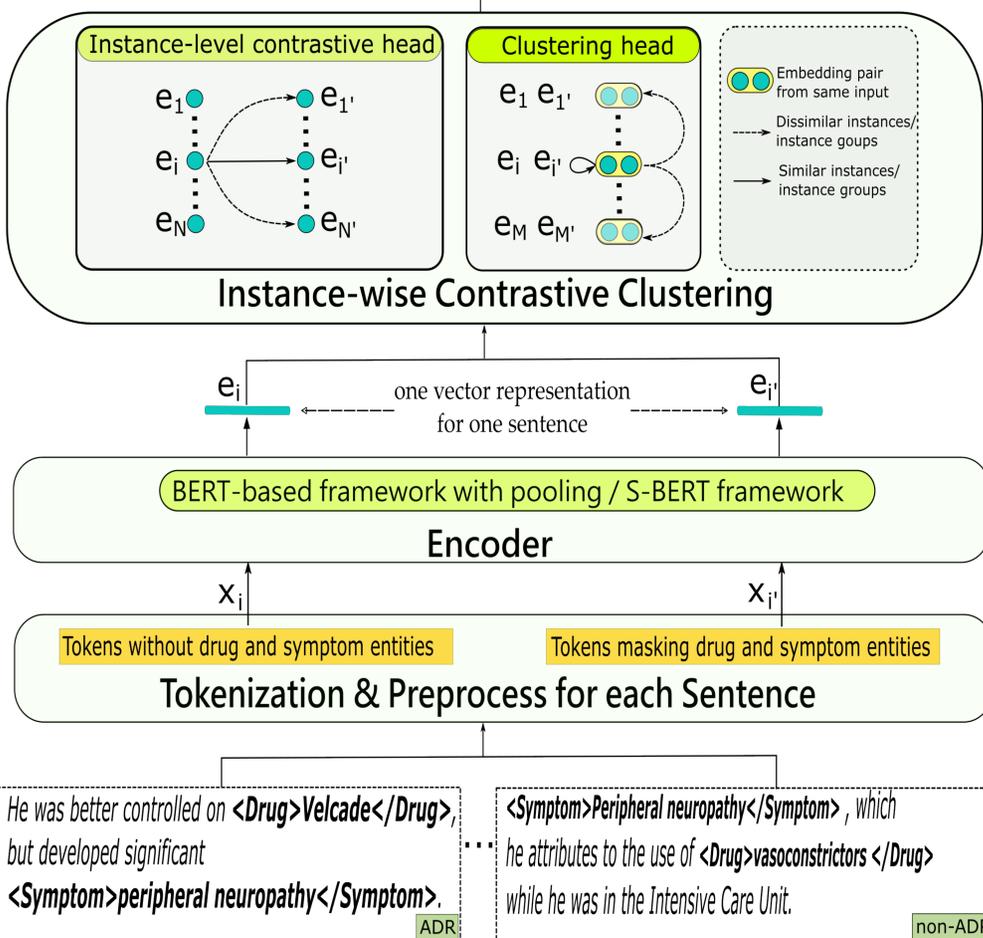
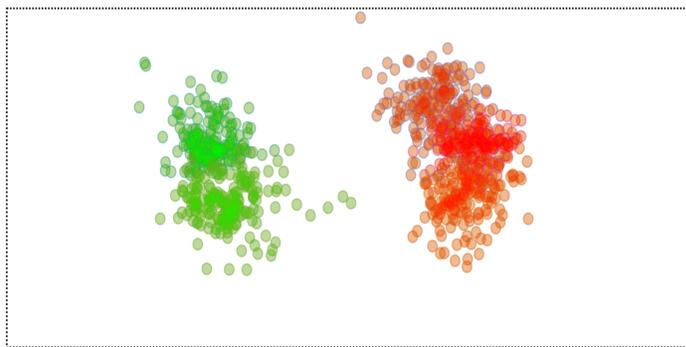
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1. Motivation

- Adverse Drug Reactions (ADRs) being mandatory for healthcare professionals, pharmacovigilance still suffers from a significant under-reporting, accounting for only 5-10% of all ADRs.
- Identification of ADRs relies on the well-trained health professionals, while there are still an enormous amount of documents waiting to be reviewed.
- Annotating such electronic health records (EHRs) is very expensive, yet supervised approaches need a large amount of annotated data.

2. Structure of Model Pipeline

- Assumption: "the ADR relation lies in the contexts of the drug-symptom target entities". More specifically, we assume there exists a short text around the entities pair which is sufficient for the representation of ADR.
- Our goal is to separate the ADR-related text blocks (noted as positive blocks β^+) from non-related ones (noted as negative blocks β^-).



- BioBERT** model is pre-trained and fine-tuned on biomedical corpora instead of employing general domain text corpora in BERT. Both BERT and BioBERT are token-wise language model.
- Sentence-BERT** applies a siamese fine-tuning structure on basic BERT model to capture features in semantic space, which transform a whole sentence directly into vector representation.

4. Contrastive Learning Enhanced Clustering (CLEC)

- For the Instance-level Contrastive head, the the model is trained to distinguish between similar and dissimilar data by evaluating the loss¹

$$\ell_i^C = -\log \frac{\exp(\text{sim}(x_i, x_{i'})/\tau)}{\sum_{j=1}^M \mathbb{1}_{j \neq i'} \exp(\text{sim}(x_i, x_j)/\tau)}$$

The Instance Contrastive Loss is $\mathcal{L}_{IC} = \sum_{i=1}^M \ell_i^C / M$

- For the clustering head, we use the Student's t -distribution² to measure the similarity between mapped point z_i and centroid μ_k :

$$q_{ik} = \frac{(1 + \|z_i - \mu_k\|^2 / \alpha)^{-\frac{\alpha+1}{2}}}{\sum_{k'} (1 + \|z_i - \mu_{k'}\|^2 / \alpha)^{-\frac{\alpha+1}{2}}}$$

and refine the clusters with the help of an auxiliary target distribution³ $p_{ik} = \frac{q_{ik}^2 / f_k}{\sum_{k'} q_{ik}^2 / f_{k'}}$ with $f_k = \sum_i q_{ik}$ as soft cluster frequencies,

The objective is a KL divergence loss between the soft assignments q_i and the auxiliary distribution for both instance pairs:

$$\mathcal{L}_C = \sum_{(i,i')} \ell_i^C / M + \ell_{i'}^C / M, \text{ where } \ell_i^C = \sum_j \sum_k p_{ik} \log \frac{p_{ik}}{q_{ik}}$$

- Total objective of CLEC: $\mathcal{L}_{CLEC} = \mathcal{L}_{IC} + \eta \mathcal{L}_C$.

5. Results and Discussion

Experimental Data

- Data source from MADE challenge 2018, whose corpora are only electronic health records.
- The information about medications and symptoms are given.
- MADE 1d1s** where we extract those who has exactly one drug and one symptom as the "perfect situation", a nearly balanced dataset with short textual blocks.
- MADE multi-d-s** has longer blocks of the EHR corpus with an almost balanced distribution between negative and positive blocks. Each block contains at least one drug and one symptom.
- In BioBERT based model, we use average pooling for short text input in **MADE 1d1s** and took [CLS] representation for long inputs in **MADE multi-d-s**

We have chosen a fully supervised approach (Bag of Words + Logistic Regression Classifier) as the upper bound baseline, and a BoW with random guessing as the lower bound.

The results for unsupervised approaches (*) are always followed by a KMedoids clustering

Category	Exp	MADE 1d1s		
		Prec	Recall	F1
Supervised	BOW+LR	0.702	0.797	0.746
Unsupervised	BioBERT* ⁴	0.651	0.663	0.650
	SBERT* ⁴	0.733	0.615	0.665
Unsupervised	BioBERT+CLEL	0.768	0.669	0.715
	SBERT+CLEL	0.646	0.711	0.677
Supervised	BOW+Random	0.514	0.529	0.522

Category	Exp	MADE multi-d-s		
		Prec	Recall	F1
Supervised	BOW+LR	0.809	0.847	0.827
Unsupervised	BioBERT* ⁴	0.604	0.634	0.619
	SBERT* ⁴	0.653	0.673	0.663
Unsupervised	BioBERT+CLEL	0.582	0.827	0.673
	SBERT+CLEL	0.660	0.773	0.702
Supervised	BOW+Random	0.509	0.440	0.472

- Both BioBERT-based model and SBert-based Model benefit the contrastive clustering comparing to our previous work.

- For short EHR data, BioBERT based model benefits more from its biomedical domain specified dictionary comparing to

the SBERT-based model,

- SBert model has more advantage for long textual EHR data,

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