Bachelorarbeit Verteidigung

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Studiere Zukunft

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Thema

Transformer Based Medication Prediction from Clinical Notes

Thema

Wozu?

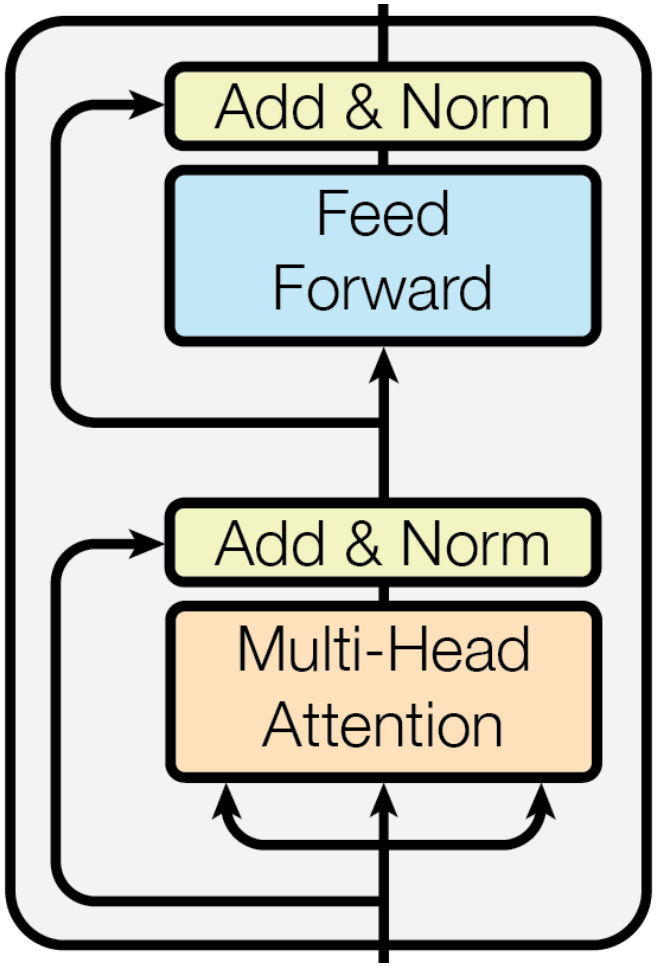
- Ärtz*innen haben wenig Zeit
- viele Medikamente und Krankheiten
- komplexe Entscheidungen + wenig Zeit = Schwierig
- Lösung: Automatisierte Vorschläge

Hintergrund

1. BERT
2. Bi-Encoder
3. Clinical Outcome Prediction
4. Medication Prediction

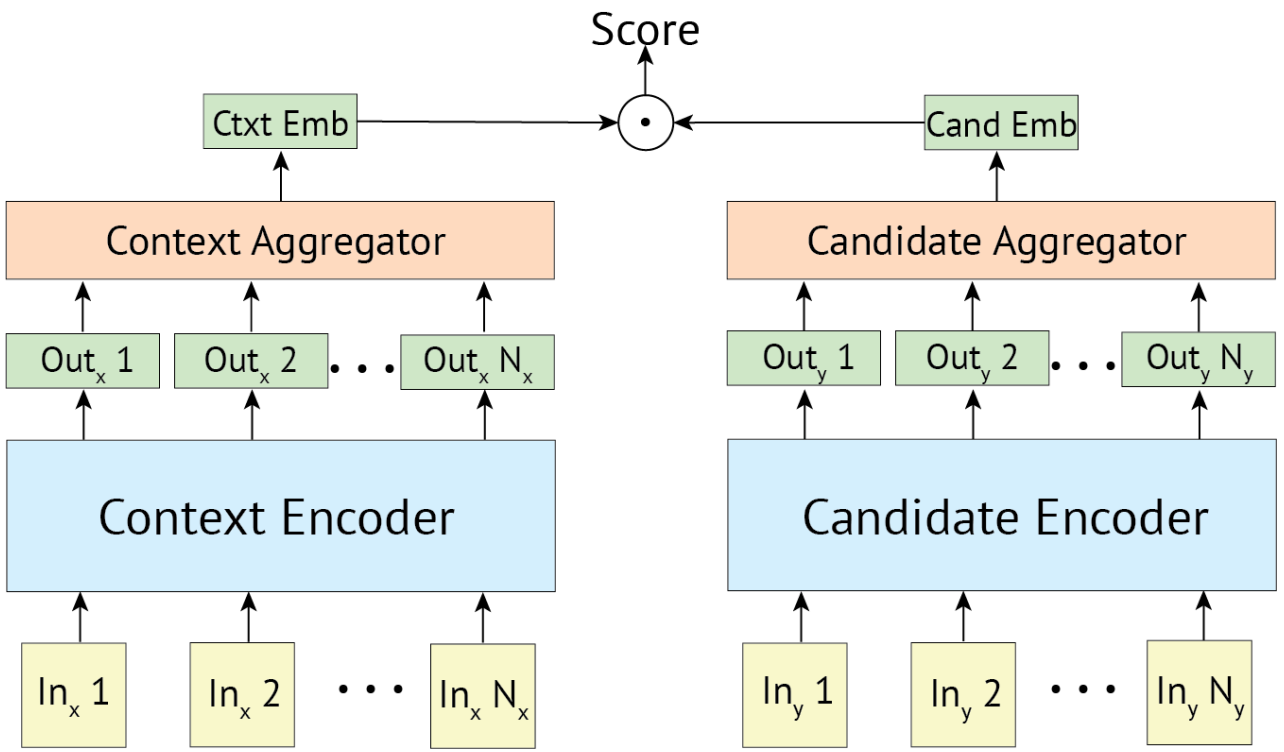
BERT

- Devlin et al. (2019)
- Nutzt Transformer-Encoder-Layers (Vaswani et al. (2017))
- Pretraining
- Finetuning
- BioBERT (Lee et al. (2019))



Bi-Encoder

- Humeau et al. (2020)
- Zwei Encoder
- Embeddings annähern durch Training



Clinical Outcome Prediction

- Verwand mit Medication Prediction
- Vorhersagen von klinischer Behandlung mithilfe von Patientenrepräsentation
- Textuelle Patientenrepräsentation (van Aken et al (2021), Zhang et al. (2020))

Medication Prediction

- Wenige veröffentlichungen
- Vorhersage von Haupt- und Nebenwirkungen (Jang et al. (2018), Wu et al. (2019))
- Auf Basis von Krebs DNA (Baptista et al. (2020), Kim et al. (2020))
- Auf Basis ICD-Code-Sequenz (Choi et al. (2016), Liu et al. (2020), Song et al. (2021))
- Keine textuelle Patientenrepresentation

Methodik

- Definition des Tasks
- Daten
- Ansätze

Definition des Tasks

- Vorhersage von Medikamenten
- Auf Basis von textueller Patientenrepräsentation
- Fokus auf Wirkstof

Daten

- MIMIC-III (Johnson et al. (2016))
- Admission Notes (van Aken et al. (2021))
- Wikipedia
- Trigram Fuzzy Matching

Ansätze

- BERT-Basierter Classifier
- BERT-Basierter Bi-Encoder

Classifier

- BERT-Classifier (Devlin et al. (2019))
- BioBERT
- Drug Classifier (Admission Note => Drug Name)
- Article Classifier (Admission Note => Linked Wikipedia Article)
- Training mit und ohne Long-Tail

Bi-Encoder

- BERT-Encoder (BioBERT)
- Dot-Product Similarity
- Single Label Loss (crossentropy)
- Multi Label Loss (binary crossentropy)
- Mit und ohne Long-Tail

Single Label Loss		
Aspirin		
Paracetamol		
Multi Label Loss		
Aspirin		
Paracetamol		

Auswertung

- Hyphothesen
- HPO
- Experimente
- Vergleich Classifier und Bi-Encoder

Hyphothesen

- Bi-Encoder besser als Classifier
- Training mit Long-Tail schlechter
- Multi-Label Bi-Encoder besser als Single-Label
- Recall besser als Precision
- Größere Batch-Sizes Besser

HPO Classifier

- Batch-Sizes kein signifikanter Unterschied

Model	Batch Size	Learning Rate
Drug Classifier	16	$4 \cdot 10^{-5}$
Drug Classifier All	16	$4 \cdot 10^{-5}$
Article Classifier	32	$4 \cdot 10^{-5}$
Article Classifier All	32	$4 \cdot 10^{-5}$

HPO Bi-Encoder

- Größere Batch-Sizes funktionieren besser
- Sigmoid funktioniert deutlich schlechter

Model	Batch Size	Learning Rate	Activation Function
Bi-Encoder	16	$4 \cdot 10^{-5}$	mish
Bi-Encoder All	16	$4 \cdot 10^{-5}$	mish
Bi-Encoder MC	32	$4 \cdot 10^{-5}$	mish
Bi-Encoder MC All	32	$4 \cdot 10^{-5}$	mish

Experimente Classifier

- Beste Resultate um Bester AUROC Wert
- Varianten mit Long-Tail nicht signifikant schlechter
- Precision bessert als Recall

Model	Accuracy	Precission	Recall	F1	AUROC
Drug Classifier	0.9735	0.7550	0.4165	0.5123	**0.8392**
Drug Classifier All	**0.9940**	0.7000	0.4294	0.5080	0.7799
Article Classifier	0.9224	**0.7604**	**0.5371**	**0.6135**	0.8112
Article Classifier All	0.9799	0.7590	0.5208	0.5972	0.8083

Experimente Bi-Encoder

- Beste Resultate um besten NDCG Wert

Model	AUROC	Recall@1	Recall@5	Recall@10	Recall@32	NDCG
Bi-Encoder	0.6675	0.3888	0.3394	0.3234	0.4219	0.6614
Bi-Encoder All	0.6853	0.3294	0.2669	0.2278	0.1932	0.5270
Bi-Encoder MC	**0.7666**	**0.9550**	**0.8599**	**0.7780**	**0.7282**	**0.8870**
Bi-Encoder MC All	0.7474	0.9514	0.8584	0.7766	0.6454	0.8523

Vergleich Classifier und Bi-Encoder

- Drug Classifier nicht vergleichbar
- Clasifier Besser als Bi-Encoder

Model	AUROC
Article Classifier	**0.8112**
Bi-Encoder	0.6675
Bi-Encoder MC	0.7666
Article Classifier All	**0.8083**
Bi-Encoder All	0.6853
Bi-Encoder MC All	0.7474

Zusammenfassung

- Bi-Encoder schlechter als Classifier
- Long-Tail nur unsignifikant schlecher
- Multi-Label Loss Bi-Encoder besser als Single Label
- Precision besser als Recall
- Größere Bi-Encoder Batch-Sizes besser
- Bi-Encoder deutlich schlechter mit sigmoid

Ausblick

- Andere Architekturen (Poly-Encoder, Cross-Encoder) (Humeau et al. (2020))
- Bessere Quelle für Medikament Beschreibungen (DailyMed(FDA))
- Mehr Aktivirungsfunktionen für Bi-Encoder
- Dosierung
- Längere Texte (Beltagy et al. (2020), Kitaev et al. (2020))
- Bessere Verknüpfung von Medikamenten

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Fragen?