Fine-Tuning Pretrained Language Models With Label Attention for Biomedical Text Classification

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Abstract

The massive scale and growth of textual biomedical data have made its indexing and classification increasingly important. However, existing research on this topic mainly utilized convolutional and recurrent neural networks, which generally achieve inferior performance than the novel transformers. On the other hand, systems that apply transformers only focus on the target documents, overlooking the rich semantic information that label descriptions contain. To address this gap, we develop a transformer-based biomedical text classifier that considers label information. The system achieves this with a label attention module incorporated into the fine-tuning process of pretrained language models (PTMs). Our results on two public medical datasets show that the proposed fine-tuning scheme outperforms the vanilla PTMs and state-of-the-art models.

1 Introduction

Clinical practices and biomedical research generate a vast and rapidly growing amount of textual data (Dash et al., 2019). This includes written information about patients in electronic health records (EHRs) and millions of articles recorded by biomedical research databases. To analyze this magnitude of data effectively, we need large-scale organization and classification (Botsis et al., 2011). However, such schemes (e.g., medical coding, medical subject headings (MeSH) indexing) mainly employ specially educated professionals for manual classification. Not only is this approach expensive, but it has also been shown to be unreliable (Dai et al., 2020; Omalley et al., 2005). As a result, automated medical text indexing and classification systems have been an active research area in recent years.

Recent works in this area have primarily focused on convolutional and recurrent neural network-based architecture and word embeddings (e.g., word2vec, fastText, and ELMo). For example, the ML-NET (Du et al., 2019) comprises an RNN-based architecture with ELMo embeddings and a label count prediction module. CAML (Mullenhbach et al., 2018) utilizes the word2vec embedding and CNNs for document encoding and the dot-product label attention mechanism for injecting label information. Compared to such architectures, transformer-based pretrained language models (PTMs) such as BERT and GPT-3 have achieved great performance gains, dominating leaderboards in most natural language processing tasks. However, studies that apply PTMs based on transformers in bioinformatics have mainly worked on improving the pretraining process with better data and techniques (Wu et al., 2019). This forgoes the valuable information labels contain, especially in the medical context.

In this paper, we propose a novel neural network architecture that involves fine-tuning biomedical versions of the BERT language model (Devlin et al., 2019; Lee et al., 2019) with label attention for explainable biomedical text classification. We name our method Label Attention Modeling for
Explainability (LAME)\textsuperscript{1}. Our motivations for the design are three-fold: (1) BERT, a state-of-the-art (SOTA) transformer-based PTM, generates a more accurate representation of biomedical texts; (2) fine-tuning it, instead of performing feature extraction, leads to better results, as shown by Peters et al. (2019); (3) label attention helps attend to n-grams in documents relevant to the label. Moreover, the label attention module can explain the prediction via attention scores, thus giving us insights into the system’s decision-making process. This interpretability is critical in medical sciences, differentiating our model from most deep learning approaches. We conduct experiments on two public biomedical datasets and show that our approach outperforms the conventionally fine-tuned BERT, a feature extraction-based BERT with label attention, and the SOTAs in both instances.

2 Method

This paper formulates the LAME fine-tuning architecture for the multi-class and multi-label classification settings. Let the set of all labels be \( \mathcal{L} \). Given the input sequence \( \mathbf{x} \), the model determines the probability of class or label \( y_\ell \) for all \( \ell \in \mathcal{L} \) based on the \( \mathbf{u}_\ell \) label description representation. Figure 2 shows the design of both the model and the label description embedding process. In detail, the target sequence and the label descriptions are first passed into the pretrained BERT model, resulting in deep contextualized representations. Then, our label attention layer helps the label descriptions attend to important locations within the sequence. The output is aggregated and normalized with a feedforward layer and a softmax/sigmoid function to get the final class/label probabilities.

2.1 Fine-tuning biomedical BERT

BERT, introduced by Devlin et al. (2019), generates deeply bidirectional contextualized representations of language. It achieves this with a stacked Transformer encoder structure (Vaswani et al., 2017) and advanced pretraining tasks such as masked language modeling and next sentence prediction. To adapt to different domains, BERT can be flexibly fine-tuned or pretrained on in-domain textual data. We choose to fine-tune the BioBERT (Lee et al., 2019) variant—which was specifically created for biomedical NLP—because of its empirical performance on the experimented datasets. We refer to it in our design only as BERT for the convenience of notation.

As the input of BERT in the model, we have the target document sequence \( \mathbf{x} = \{x_1, x_2, ..., x_N\} \), where \( N \) is the length of the document. Let \( \mathbf{H}^l \) be the representation created at the \( l \)-th Transformer encoder layer of BERT, where \( l \in [1, L] \), and \( d_h = 768 \) is the hidden dimension hyperparameter. The process can be formulated as follow:

\[
\mathbf{H}^l = \text{TransformerEncoder}_l(\mathbf{H}^{l-1}),
\]

where \( \mathbf{H}^0 \) is the input embeddings of \( \mathbf{x} \). The output is the matrix representation \( \mathbf{H}^L \in \mathbb{R}^{N \times d_h} \) of the target document sequence. We call it by the shorthand notation \( \mathbf{H} \).

2.2 Label Description Embedding

For each label \( \ell \), we input its description into the pretrained BERT to obtain its representation vector \( \mathbf{u}_\ell \in \mathbb{R}^{d_h} \). This is done by taking the final hidden state \( \mathbf{h}_L^{[\text{CLS}]} \) of the special [CLS] token for classification tasks. We repeat this step for every training instance \( i \) and thus fine-tune the model’s parameters concerning the label representation. As a result, the pretrained BERT jointly learns the most appropriate representations for both the document \( \mathbf{x} \) and the label \( \ell \). All the label representation vector \( \mathbf{u}_\ell \) with \( \ell \in \mathcal{L} \) is then concatenated into matrix \( \mathbf{U} \in \mathbb{R}^{|\mathcal{L}| \times d_h} \) for further processing by the label attention layer.

2.3 Label Attention Layer

Our design of this layer is inspired by the Transformer model architecture (Vaswani et al., 2017) and its immense success in modeling language dependency. The layer comprises a multi-head attention sub-layer and a feedforward network, with residual connections (He et al., 2016) and layer normalization schemes (Ba et al., 2016) after each sub-layer. We choose multi-head attention instead of conventional attention modules because we hypothesize that it is more effective in high-dimensional space of \( \mathbf{H} \in \mathbb{R}^{N \times d_h} \) and \( \mathbf{U} \in \mathbb{R}^{|\mathcal{L}| \times d_h} \). In addition, it is possible to stack blocks of label attention to produce a deeper cross attention signal between the target document and the labels.

In details, we have the output of each sub-layer as \( \text{LayerNorm}(\mathbf{x} + \text{Sublayer}(\mathbf{x})) \) where \( \mathbf{x} \) is the input and Sublayer is the operation performed by each sub-layer (multi-head attention and fully connected network). At the base of the module, the

\textsuperscript{1}The source code will be made available.
target document representation matrix \( \mathbf{H} \) and the label embedding space \( \mathbf{U} \) are fed into the multi-head attention layer. The former represent the key and value and the latter the query for the subsequent scaled dot-product attention calculation:

\[
\mathbf{O} = \text{Attention}(\mathbf{U}, \mathbf{H}, \mathbf{H}) = \text{softmax}\left(\frac{\mathbf{U} \mathbf{H}^T}{\sqrt{d_h}}\right) \mathbf{H},
\]

where \( \mathbf{O} \in \mathbb{R}^{|L| \times d_h} \) is the attention output. Since we are using multi-head attention, the actual underlying operations are as follows:

\[
\text{head}_i = \text{Attention}(\mathbf{UW}_i^Q, \mathbf{HW}_i^K, \mathbf{HW}_i^V),
\]

\[
\text{MultiHead}(\mathbf{U}, \mathbf{H}, \mathbf{H}) = \text{Concat}(\text{head}_i) \mathbf{W}_O^O
\]

for all \( i \in [1, h] \), where \( \mathbf{W}_i \) and \( \mathbf{W}_O \) are the projection parameter matrices. Regarding the number of heads, we adopt \( h = 12 \) based on analyses by (Voita et al., 2019) and our experimental results. After calculating attention scores, the attention output \( \mathbf{O} \) is aggregated with \( \mathbf{U} \) and normalized. The resulting matrix is then passed onto the next sub-layer, keeping its dimensions unchanged throughout the process.

2.4 Classification & Loss Function

Let \( \mathbf{O} \in \mathbb{R}^{|L| \times d_h} \) be the final output of the label attention layer(s). It is then further fed into another feedforward network and finally, the softmax (for multi-class classification) or sigmoid (for multi-label classification) function to obtain the final label probabilities \( y_\ell \) for all \( \ell \in L \).

For biomedical multi-class text classification, we employ the prevalent cross-entropy loss. Unfortunately, in the multi-label case, there is often a substantial degree of imbalance within the datasets, making the commonly-used binary cross-entropy loss suboptimal (Eban et al., 2017). Therefore, we also experiment with a loss function based on the F-measure for mini-batch training:

\[
L_{F\text{-measure}} = \frac{1}{2} \left( \frac{2p}{2p + (fp + fn)} + \frac{2n}{2n + (fp + fn)} \right)
\]

with \( tp, tn, fp, fn \) being the true positive, true negative, false positive, and false negative micro-
weighted rates within a mini-batch. In our experiments, we find that while this loss does not improve the fine-tuning process of base BERT, it helps with the convergence of LAME.

3 Experiments

3.1 Datasets & Baselines

We train LAME following the setup of previous SOTA methods on two biomedical datasets: (1) Hallmarks of Cancers (HoC) \(^2\) (Baker et al., 2016): a multi-label dataset with 1,580 PubMed abstracts labeled with the 10 hallmarks of cancer. We split this dataset into train/dev/test sets with a ratio of 7:1:2. (2) Medical abstracts of diseases (Disease-5) \(^3\): a multi-class dataset with 14,102 medical abstracts falling into 5 classes. We split the dataset into train/dev/test sets with a ratio of 8:1:1. Since the label descriptions of Disease-5 are not given, we create our own according to our best knowledge. We take into account previous works while also building our baselines for comparisons. For HoC and Disease-5, we include the ML-NET and the BiForest model (Wang et al., 2019) as the SOTA, respectively. The latter used a tree-structured LSTM and the attention mechanism for more explainable predictions. The authors in both studies also presented a single-layer one-dimensional CNN baseline (Kim, 2014), which we also utilize for comparisons. In addition to LAME, we experiment with a typically fine-tuned BERT for text classification (Sun et al., 2019), and a feature extraction-based approach to BERT (frozen BERT) (Peters et al., 2019), which has a CNN as the classification head. Unfortunately, we find that stacking label attention does not yield performance gains, possibly because of the small size of both datasets. Therefore, their performances are not included in the study.

3.2 Hyperparameters & Evaluations

We experiment with a batch size of 42, 1 and 4 NVIDIA A100 GPUs for the HoC and Disease-5, respectively. A slanted triangular learning rate (Howard and Ruder, 2018) with 0.1 warm-up portions is used for BERT and label attention with a 5e-05 and 4e-02 respective maximum learning rate. The classification head’s learning rate, on the other hand, stays unchanged at 1e-03 for the whole 30 epochs of training. The optimizer used is AdamW (Loshchilov and Hutter, 2019). We use micro-weighted F-score, precision, and recall for evaluation in the HoC task, while performance in Disease-5 is only evaluated using accuracy, following Wang et al. (2019).

3.3 Results

Results show that our model achieves a noticeable improvement over all the baselines. Most significantly, LAME outperforms conventionally fine-tuned BERT by approximately 0.3 in F1 in the HoC and 0.5 in accuracy level in the Disease-5 task, showing that injecting label information into the fine-tuning process improves performance. At the same time, the fine-tuned transformer-based methods are shown to be superior to feature extraction-based ones, with the success of fine-tuned BERT variants.

3.4 Interpretability

Given an example \(x\) and an output prediction \(\ell\), we can extract the attention scores \(\alpha_\ell\) generated by the multi-head attention layer within the label attention network. By aligning this vector \(\alpha_\ell\) with the input list of tokens, we find the tokens that influence the decision of the model the most. Figure 1 shows an example of the results. Since BERT employs the WordPiece tokenizer, out-of-vocabulary or rare tokens are divided into subwords. Therefore, the attention can be on such subwords, as evident in the figure. Readers interested in quantitative interpretability analyses of the label attention module can refer to the extensive study by Mullenbach et al. (2018).

4 Conclusion

This paper devises a new deep learning architecture to solve the biomedical text classification task. This approach involves fine-tuning a pretrained BERT language model with a label attention module. Therefore, it can learn rich representations of input texts while accounting for the label description information. Results show the effectiveness of this approach against many baselines and existing methods. Furthermore, we can interpret the model’s decisions thanks to the attention mechanism. In doing this, we hope to further the use of deep learning in bioinformatics by shedding light on these powerful black-box neural networks.
References

Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. 2016. Layer normalization. arXiv preprint arXiv:1607.06450.

Simon Baker, A. Korhonen, and Sampo Pyysalo. 2016. Cancer hallmark text classification using convolutional neural networks. In BioTxtM@COLING 2016.

Taxiarchis Botsis, Michael D Nguyen, Emily Jane Woo, Marianthi Markatou, and Robert Ball. 2011. Text mining for the vaccine adverse event reporting system: medical text classification using informative feature selection. Journal of the American Medical Informatics Association, 18(5):631–638.

Suyang Dai, Ronghui You, Zhiyong Lu, Xiaodi Huang, Hiroshi Mamitsuka, and Shanfeng Zhu. 2020. Fullmesh: improving large-scale mesh indexing with full text. Bioinformatics, 36(5):1533–1541.

Sabyasachi Dash, Sushil Kumar Shakyawar, Mohit Sharma, and Sandeep Kaushik. 2019. Big data in healthcare: management, analysis and future prospects. Journal of Big Data, 6(1):1–25.

J. Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. 2019. Bert: Pre-training of deep bidirectional transformers for language understanding. In NAACL.

Jingcheng Du, Qingyu Chen, Yifan Peng, Yang Xiang, Cui Tao, and Zhiyong Lu. 2019. Mi-net: multi-label classification of biomedical texts with deep neural networks. Journal of the American Medical Informatics Association, 26(11):1279–1285.

Elad Eban, Mariano Schain, Alan Mackey, Ariel Gordon, Ryan Rifkin, and Gal Elidan. 2017. Scalable learning of non-decomposable objectives. In Artificial intelligence and statistics, pages 832–840. PMLR.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. 2016. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 770–778.

Jeremy Howard and Sebastian Ruder. 2018. Universal language model fine-tuning for text classification. In ACL.

Yoon Kim. 2014. Convolutional neural networks for sentence classification. In EMNLP.

J. Mullenbach, Sarah Wiegreffe, J. Duke, Jimeng Sun, and Jacob Eisenstein. 2018. Explainable prediction of medical codes from clinical text. In NAACL.

Kimberly J. Omalley, Karon F. Cook, Matt D. Price, Kimberly Rafterd Wildes, John F. Hurdle, and Carol M. Ashton. 2005. Measuring diagnoses: Icd code accuracy. Health Services Research, 40(5p2):1620–1639.

Matthew E. Peters, Sebastian Ruder, and Noah A. Smith. 2019. To tune or not to tune? adapting pretrained representations to diverse tasks. In RepL4NLP@ACL.

Chi Sun, Xipeng Qiu, Yige Xu, and Xuanjing Huang. 2019. How to fine-tune bert for text classification? In China National Conference on Chinese Computational Linguistics, pages 194–206. Springer.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. 2017. Attention is all you need. In Advances in neural information processing systems, pages 5998–6008.

Elena Voita, David Talbot, F. Moiseev, Rico Sennrich, and Ivan Titov. 2019. Analyzing multi-head self-attention: Specialized heads do the heavy lifting, the rest can be pruned. In ACL.

ZhiGuo Wang, Y. Zhang, Mo Yu, Wei Zhang, Lin Pan, Linfeng Song, Kun Xu, and Y. El-Kurdi. 2019. Multi-granular text encoding for self-explaining categorization. In BlackboxNLP@ACL.

Stephen Wu, Kirk Roberts, Sarabhi Datta, Jingcheng Du, Zongcheng Ji, Yuqi Si, Sarvesh Soni, Qiong Wang, Qiang Wei, Yang Xiang, and et al. 2019. Deep learning in clinical natural language processing: a methodical review. Journal of the American Medical Informatics Association, 27(3):457–470.