Classification of Scientific Research Articles Using Large Language Models

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Overall setting

The following document is a description of my solution to the Arxiv research papers classification assignment. In the next sections I describe how the dataset was preprocessed, present insights from an initial investigation of of the data, the formal definition of a machine learning task, and the machine learning models that I developed.

Dataset

The dataset consists of research papers uploaded to the online research repository arxiv.org from 2008 onward. In total, there are above 1,7 million research papers. Each paper is assigned or more categories to which the paper belongs. The dataset is publicly available and described in more details here: https://www.kaggle.com/datasets/Cornell-University/arxiv

Subsampling

As the data is massive and it is unfeasible to run a large language model on the full dataset, I worked with a small sample of the data. In order to mimic a real-life application setting, I sampled 10% of the papers from 2021 as a training dataset and I sampled 10% from the papers in the first half of 2022 for validation, and the test set consists of 10% of the papers published on arxiv in the second half of 2022.

Labeling

The total number of all categories and subcategories is rather large, above 150, hence I consider only the main categories that correspond to different scientific disciplines. This results in 21 unique labels.

In Figure 1 I show the distribution of labels in the train dataset. In Figure 2, as a sanity check, I show the label distribution in the validation and test sets. As the distribution is skewed, we should consider different evaluation metrics that address the skewness in an informative way. We discuss this in the next sections.

Each research paper is assigned one or more categories. Usually, these are subcategories of the same main category, such as 'cs.DM' and 'cs.IR', but for many papers there are several categories. In Figure 3 I show the number of labels per paper (for the detected "general" 21 labels). Clearly, the number of papers with more than one label is significant, thus we have a *multiclass multilabel* problem. This needs to be addressed in the design and evaluation of the prediction models.

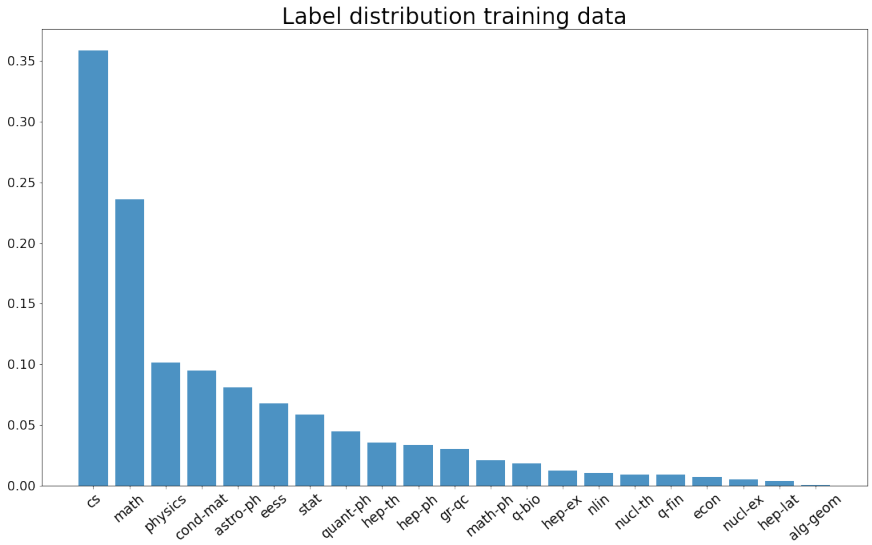

Figure 1: The distribution of labels in the training dataset.

Research overview

The problem is a classic classification task for which I used a precomputed Bert model [2], so I mostly used online tutorials, and Keras/Tensorflow and Hugging Face documentation, Andrew Ng's lecture notes on sequential neural network models, machine learning forums, etc. [1, 5]. The techniques used in the implementation are more or less standard. But due to a large number of parameters, the precise solution had to be carefully chosen, so I had to investigate practical advices on the definition of the problem. The only new research paper I read was on the Focal Loss [4], an extension the classic CrossEntropy loss such that the loss adjusts itself to assign more importance to examples with less confident prediction. A more thorough discussion can be found in the corresponding section below.

The classification model

Here I present models that address the classification task. As already explained, I consider a multiclass multilabel classification problem. (I also implemented a model where we consider only the first category of the paper and we have a standard single-label multiclass setting with a softmax output payer in a neural network model but I don't report results on it due to lack of time.)

I designed models that predict the paper label using the paper's abstract. Other features present in the data, such as the paper title or the authors, were not used but in principle should be considered in order to design more powerful models.

In the next sections I describe three models I implemented. The first one is a baseline model that only uses the word distributions, the second one is a deep learning model that uses transfer learning from a pretrained large language Bert model. The third model builds upon the second one by incorporating an LSTM layer in the model.

Technical aspects The dataset is very large and applying a large language model to it would require considerable computational resources. Furthermore, I don't own a GPU and decided to use to publicly available Kaggle GPUs. However, there are certain time constraints on the usage of GPUs in Kaggle notebooks.

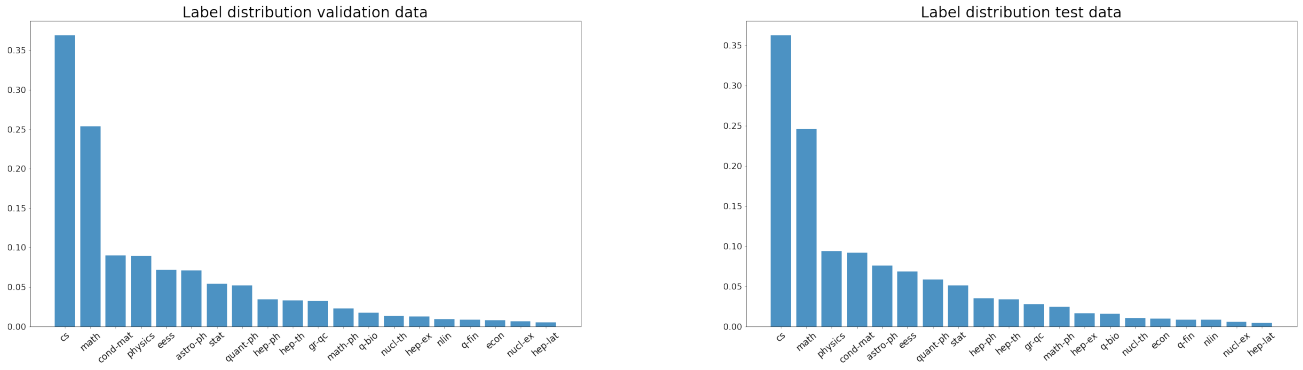

Figure 2: The distribution of labels in the validation and test datasets.

Hence, as I explained, I decided to work with a small sample of the data. Furthermore, I used smaller neural network models that can be trained and evaluated in reasonable time.

Baseline model

As a baseline model, I implemented CountVectorizer that generates word frequency vectors that represent the abstracts. Then I predicted the paper category using a simple Decision tree model by selecting the optimal tree depth using the validation dataset.

Deep learning models

The overall architecture is shown in Figure 4. After tokenization of the paper's abstract, we are using the precomputed token embeddings as a static lookup table, i.e., the embedding layer is frozen and the weights are not fine-tuned during training. This is done in order to ensure more scalable training and finish the task on time. Then the token embeddings are aggregated using max-pooling operator. (I also tried average pooling and the results were worse but I didn't test it extensively.)

As a second, slightly more advanced architecture I used an LSTM layer with trainable parameters for aggregation of the token embeddings, instead of the pooling aggregation, this is an aggregation method presented in [3].

The loss function It is standard to use the binary cross-entropy loss for multilabel problems. Thus, the output layer of the network has sigmoid as the activation function and returns the probability for each of the considered classes. As an alternative to cross-entropy I also ran experiments using Focal loss [4]. See the next section for more details.

Regularization. I use Dropout and early stopping on the validation set for regularization of the model. As metrics, I used AUC and the F1-score with probability threshold 0.5, see Figures 5 and 6.

Focal Loss

The classic cross-entropy function is defined as

$$CE(y, \tilde{y}) = \frac{1}{n} \sum_{i=1}^{n} -y_i \log \tilde{y}_i - (1 - y_i) \log(1 - \tilde{y}_i)$$

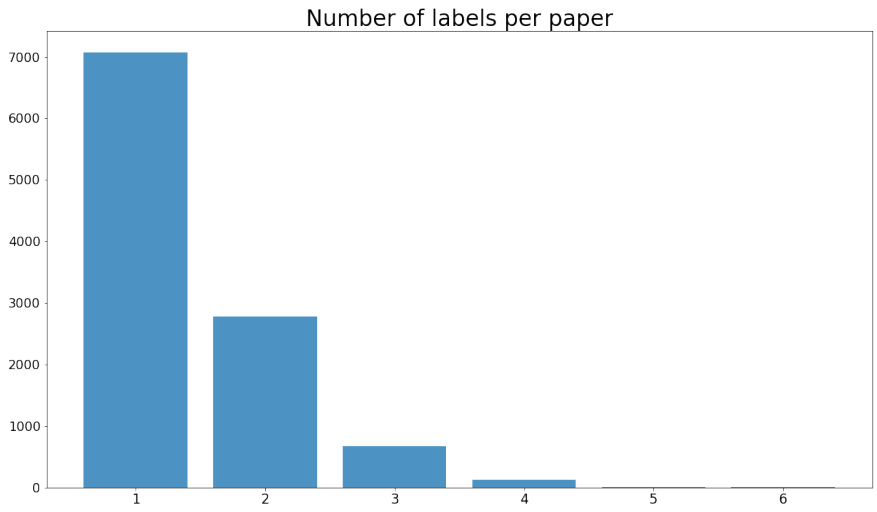

Figure 3: The number of distinct labels per paper in training dataset.

where y_i and $\tilde{y}_i$ are the actual and predicted labels, respectively. The above is extended with the so called local factor $(1 - y_i)^\gamma$ for the positive class, for some $\gamma \geq 0$ [4]. Thus, the function becomes

$$FocalLoss(y, \tilde{y}) = \frac{1}{n} \sum_{i=1}^{n} -y_i(1 - \tilde{y}_i)^\gamma \log \tilde{y}_i - (1 - y_i)\tilde{y}_i^\gamma \log(1 - \tilde{y}_i)$$

For $\gamma = 0$ we have the standard cross-entropy. The larger γ leads to assigning less weight to highly confidential predictions. For example, if the true label $y_i = 1$ and the model predicts $\tilde{y}_i = 0.99$, we discount the contribution of the prediction by a factor of 0.01^γ. For a less confident prediction, e.g., $\tilde{y}_i = 0.8$, the discount factor is 0.2^γ, i.e., the model should pay more attention to such "less confident" examples. It is argued that this is a remedy for class imbalance as the infrequent classes often exhibit more specific feature patterns.

I use the Focal Binary CrossEntropy Loss with the default value $\gamma = 2$.

Results

The results after evaluating the models on the test dataset are summarized in Table 1. We use the micro and macro variations of the AUC and F1 scores. The micro average of a given metric μ considers all examples equally important, while the macro averages the values over classes independent of the cardinality of the class:

$$\text{micro-avg}(\mu) = \frac{1}{n} \sum_{i=1}^{n} \mu(y_i, \tilde{y}_i)$$

Let C be the number of all classes and let n_c be the number of example in a given class c.

$$\text{macro-avg}(\mu) = \frac{1}{C} \sum_{c=1}^{C} \left(\frac{1}{n_c} \sum_{i=1}^{n_c} \mu(y_i, \tilde{y}_i) \right)$$

```
Model: "model"
__________________________________________________________________________________________________
 Layer (type)                   Output Shape         Param #     Connected to
==================================================================================================
 input_ids (InputLayer)         [(None, 512)]        0           []

 attention_mask (InputLayer)    [(None, 512)]        0           []

 tf_bert_model (TFBertModel)    TFBaseModelOutputWi  109482240   ['input_ids[0][0]',
                                thPoolingAndCrossAt               'attention_mask[0][0]']
                                tentions(last_hidde
                                n_state=(None, 512,
                                 768),
                                 pooler_output=(Non
                                e, 768),
                                 past_key_values=No
                                ne, hidden_states=N
                                one, attentions=Non
                                e, cross_attentions
                                =None)

 global_max_pooling1d (GlobalMa  (None, 768)         0           ['tf_bert_model[0][0]']
 xPooling1D)

 batch_normalization (BatchNorm  (None, 768)         3072        ['global_max_pooling1d[0][0]']
 alization)

 dense (Dense)                  (None, 128)          98432       ['batch_normalization[0][0]']

 dropout (Dropout)              (None, 128)          0           ['dense[0][0]']

 outputs (Dense)                (None, 20)           2580        ['dropout[0][0]']

==================================================================================================
Total params: 109,586,324
Trainable params: 102,548
Non-trainable params: 109,483,776
__________________________________________________________________________________________________
```

Figure 4: The structure of the model.

```python
learning_rate = 0.01
optimizer = tf.keras.optimizers.Adam(learning_rate)
#optimizer = tf.keras.optimizers.SGD(learning_rate)
losses = [tf.keras.losses.BinaryCrossentropy(), tf.keras.losses.BinaryFocalCrossentropy()]
loss = losses[1]
acc = tf.keras.metrics.BinaryAccuracy('accuracy')
auc = tf.keras.metrics.AUC()

mlp_model.compile(optimizer=optimizer, loss=loss, metrics=[macro_f1, auc])
```

Figure 5: The loss function.

We clearly observe that the baseline models performs considerably worse than the deep learning models. Also, the Focal loss indeed yields marginally better macro scores that indicate that the model indeed learns more specific features when using Focal loss.

The LSTM aggregation yields worse results. Looking at the progress of train and validation error in Figure 7, it appears that the LSTM aggragation model, which has more trainable variables, is prone to overfitting and this results in such zig-zag oscillations of the validation error. Most likely, for larger datasets this will be corrected.

Extending the model

Finally, it is worth noting that the research papers contain more meta-information such as the number of authors, number of pages, if the paper is accepted to a conference or journal, etc. These features can be incorporated as part of the model but we will have to deal with mixed data. Combining the different inputs should be done carefully as we need to ensure that different feature categories are combined in a meaningful way.

```
checkpoint_path = "/kaggle/working/training/mlp_focal_cp.ckpt"
checkpoint_dir = os.path.dirname(checkpoint_path)

# Create a callback that saves the model's weights
cp_callback = tf.keras.callbacks.ModelCheckpoint(filepath=checkpoint_path,
                                                 save_weights_only=True,
                                                 verbose=1)
```

```
es_callback = tf.keras.callbacks.EarlyStopping(patience=4, monitor='val_auc', \
                                               mode='max', restore_best_weights=True)
history = mlp_model.fit(train, validation_data=val, callbacks=[es_callback, cp_callback], epochs=20)
```

```
Epoch 1/20
200/200 [==============================] - ETA: 0s - loss: 0.0685 - macro_f1: 0.2656 - auc: 0.9110
Epoch 1: saving model to /kaggle/working/training/mlp_focal_cp.ckpt
200/200 [==============================] - 453s 2s/step - loss: 0.0685 - macro_f1: 0.2656 - auc: 0.9110 - val_loss: 0.
0337 - val_macro_f1: 0.1697 - val_auc: 0.9526
Epoch 2/20
200/200 [==============================] - ETA: 0s - loss: 0.0327 - macro_f1: 0.3021 - auc: 0.9558
Epoch 2: saving model to /kaggle/working/training/mlp_focal_cp.ckpt
200/200 [==============================] - 433s 2s/step - loss: 0.0327 - macro_f1: 0.3021 - auc: 0.9558 - val_loss: 0.
0279 - val_macro_f1: 0.2940 - val_auc: 0.9686
Epoch 3/20
```

Figure 6: Training with respective callbacks.

Method	microAUC	macroAUC	micro-F1	macro-F1
DecisionTree	0.887	0.724	0.556	0.307
Classic (CrossEntropy)	0.969	0.945	0.691	0.402
Classic (FocalCE)	0.966	0.948	0.686	0.419
LSTM (CrossEntropy)	0.965	0.935	0.685	0.312
LSTM (FocalCE)	0.883	0.849	0.301	0.212

Table 1: Accuracy metrics for the different approaches.

References

[1] Jason Brownlee. Sequence Classification with LSTM Recurrent Neural Networks in Python with Keras Available online at https://machinelearningmastery.com/sequence-classification-lstm-recurrent-neural-networks-python-keras/

[2] Jacob Devlin, Ming-Wei Chang, Kenton Lee, Kristina Toutanova. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. *NAACL-HLT (1) 2019*: 4171–4186

[3] William L. Hamilton, Zhitao Ying, Jure Leskovec. Inductive Representation Learning on Large Graphs. *NIPS 2017*: 1024–1034

[4] Tsung-Yi Lin, Priya Goyal, Ross B. Girshick, Kaiming He, Piotr Dollar. Focal Loss for Dense Object Detection. *ICCV 2017*: 2999–3007

[5] Andrew Ng. CS230 Deep Learning. Available online at https://cs230.stanford.edu/

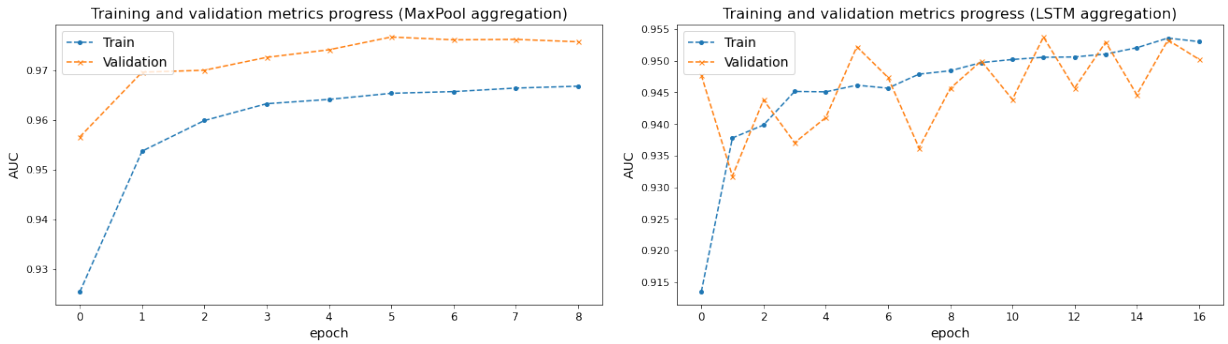

Figure 7: Training and validation loss progress for MaxPooling (left) and LSTM (right) aggregations.