Long-Tail Zero and Few-Shot Learning via Contrastive Pretraining on and for Small Data

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Abstract

For natural language processing (NLP) tasks such as sentiment or topic classification, currently prevailing approaches heavily rely on pretraining large self-supervised models on massive external data resources. However, this methodology is being critiqued for: exceptional compute and pretraining data requirements; diminishing returns on both large and small datasets; and importantly, favourable evaluation settings that overestimate performance differences. The core belief behind current methodology, coined 'the bitter lesson' by R. Sutton, is that 'compute scale-up beats data and compute-efficient algorithms', neglecting that progress in compute hardware scale-up is based almost entirely on the miniaturisation of resource consumption. We thus approach pretraining from a miniaturisation perspective, such as not to require massive external data sources and models, or learned translations from continuous input embeddings to discrete labels. To minimise overly favourable evaluation, we examine learning on a long-tailed, low-resource, multi-label text classification dataset with noisy, highly sparse labels and many rare concepts. To this end, we propose a novel 'dataset-internal' contrastive autoencoding approach to self-supervised pretraining and demonstrate marked improvements in zero-shot, few-shot and solely supervised learning performance; even under an unfavorable low-resource scenario, and without defaulting to large-scale external datasets for self-supervision. We also find empirical evidence that zero and few-shot learning markedly benefit from adding more 'dataset-internal', self-supervised training signals, which is of practical importance when retrieving or computing on large external sources of such signals is infeasible.

1 Introduction

The current prevailing approach to supervised and few-shot learning is to use self-supervised pretraining on large-scale 'task-external' data and then fine-tune on end-task labels. Recent studies have found that, thus far, this way of pretraining fails in low-resource settings (Yogatama et al., 2019; Şerbetci et al., 2020) and that reported performance improvements are caused in part by evaluation setups that are designed in line with the paradigm that "massive resources are pivotal" to improving language understanding (Linzen, 2020; Schick & Schütze, 2020a; Dodge et al., 2020; Brown et al., 2020) or computer vision (Chen et al., 2020). Despite these critiques, the underlying goal of *better initialisation of layer weights* is a core requirement of successful learning with neural networks, where self-supervised layer-wise pretraining (Bengio et al., 2006) was replaced by better layer initialisation (Glorot & Bengio, 2010), which was in turn replaced by pretraining on growing amounts of external data (Bojanowski et al., 2017; Devlin et al., 2019; Chen et al., 2020; Brown et al., 2020) – i.e. FastText, BERT, SIMCLR and GPT-3. The latter three approaches require massive compute and data resources, but enable marked learning improvements in few-shot (SIMCLR, GPT-3) or zero-shot (GPT-3) scenarios compared to models that have several orders of magnitude fewer parameters. There are also efforts to reduce model size requirements for few-shot and zero-shot adaptation by orders of magnitude (Schick & Schütze, 2020a,b; Plank & Rethmeier, 2019), with some being increasingly beneficial in scenarios with low input data (X), label resources (Y), and rare events in X. Crucially, these above-mentioned approaches do not simply rely on more data, but on creating better initialised input features X. In contrast, approaches like SIMCLR, BERT or GPT-3 (Chen et al., 2020; Devlin et al., 2019) use self-supervision via contrastive learning and input masking on large-scale datasets to create broader learning signals than supervision provides. Large-scale methods like SIMCLR rely on metric learning methods like contrastive self-supervision – i.e. learning to distinguish (dis-)similar inputs using generated, but weak supervision tasks. However, as Musgrave et al. (2020) find, "when evaluating old and recent metric learning approaches, while *controlling for data and model size*, newer methods only marginally improve over the classic contrastive formulation". Remarkably, Bansal et al. (2020) recently showed that adding broader self-supervision rather than increasing data size during large-scale pretraining can substantially boost few-shot performance.

Our central goal is thus to investigate whether *increased (broader) pretraining self-supervision also boosts few-shot and zero-shot performance using only small-scale, 'task-internal' data, in place of resorting to large-scale pretraining on two orders of magnitude more 'task-external' data (Bansal et al., 2020)* – i.e. *Do we really need large datasets for pretraining or just more (broader) self-supervised learning signals?* To broaden small data self-supervision, we propose a *contrastive self-supervised objective based on label-embedding prediction*, where labels are expressed as word embeddings to learn their matching with an input text embedding. For contrastive learning, our method samples positive and negative word input tokens X for self-supervised pretraining, zero and few-shot learning; and positive and negative classes Y for few-shot to fully supervised fine-tuning. Thus, we propose a model architecture that unifies training from labels Y and inputs X. To increase evaluation robustness, we compare models of the same parameter and data sizes as suggested by Musgrave et al. (2020), and evaluate on a challenging learning problem as suggested by Linzen (2020). Namely, we evaluate our method in challenging low-resource, long-tailed, noisy multi-label data settings, where information will always be limited, because the long tail grows with data size. For robust evaluation, we use a typical training, development, test setup and first establish a solid, fully supervised baseline for many-class multi-label classification that is optimised with a set of generalisation techniques as proposed in Jiang et al. (2020). For evaluation in supervised, few and zero-shot learning scenarios, we further analyse and then propose evaluation metric choices which are meaningful across all scenarios to allow for broader performance comparisons.

Our contributions are thus as follows. ① We provide a straight-forward method for *self-supervised contrastive label-embedding prediction* and ② evaluate it against a challenging, noisy long-tail, low-resource multi-label text prediction task. ③ We show that small-scale 'data-internal' pretraining (on 8-80MB of text) not only improves supervised performance, but also strongly boosts few and zero-shot learning by using increased self-supervision over small data, in place of resorting to the common large-scale external data pretraining approach. *This suggests that data size may matter less than signal amount, even in small data pretraining.*

2 Related Work

Large to Web-scale data pretraining is at the core of recent state-of-the-art methods in computer vision (Chen et al., 2020) and language processing (Devlin et al., 2019; Rogers et al., 2020; Brown et al., 2020). However, challenges and disadvantages are increasingly being discussed. (i) A requirement of *large-scale external data resources* (Yogatama et al., 2019; Schick & Schütze, 2020a), (ii) an inability to pretrain recent architectures on small-scale data (Liu et al., 2020; Melis et al., 2020; Şerbetci et al., 2020), (iii) calls for more challenging evaluation tasks (Linzen, 2020; McCoy et al., 2019) and (iv) diminishing returns of pretraining on large supervised datasets (Wang et al., 2020).

Challenging tasks (ii) like long-tail prediction benefit from using large-scale pretraining models (Chang et al., 2019), as do few-shot (Schick & Schütze, 2020a), or zero-shot problems, which to date require massive pretraining (Brown et al., 2020). Notably, Bansal et al. (2020) showed that rather than increased data, broader self-supervision for large-scale pretraining also boosts few-shot learning. These long-tail and few-shot learning results inspired us to investigate whether *'small data internal pretraining' similarly benefits few and zero-shot learning and whether increased self-supervision is beneficial here too – i.e. how to design pretraining for much more challenging low-resource scenarios*. Previous works have demonstrated markedly improved few and zero-shot performance by using *supervised* label embedding prediction, to either: (a) fine-tune large, externally pretrained BERT models (Chang et al., 2019); or train CNNs from scratch: on either (b) 'task-internal' data only (Pappas & Henderson, 2019), or (c) jointly over multiple supervised tasks (Zhang et al., 2018).

We combine the advantages of self-supervised pretraining and supervised label-embedding prediction in proposing an approach to *contrastive self-supervised pretraining via label-embedding prediction*. This fusion has multiple advantages: it does not require large or external resources as in (a); and its *'data-internal' self-supervision substantially boosts zero and few-shot performance without requiring task external supervised annotations* as in (b) or supervised multi-task transfer as in (c). This makes our approach *well-suited for low-resource, long-tail learning without task external labels or large-scale annotated datasets*. Finally, similar to Zhang et al. (2018); Pappas & Henderson (2019) we use CNN architectures, but modify them to be smaller and suitable for contrastive self-supervision, which also provides *a small-scale, low-resource alternative to current self-attention models* – even for challenging long-tail, low-resource scenarios. The benefits of our pretraining method and model are shown in §6.3 and §6.4, where we explore its effects on few-shot learning (*label Y-efficiency*), zero-shot learning and 'low-resource' zero-shot learning (*input X-efficiency*).

3 Dense-to-dense text prediction for contrastive autoencoding

In this section, we propose to use label-embeddings, previously used for supervised learning only (Pappas & Henderson, 2019; Zhang et al., 2018), and exploit them for *self-supervised contrastive pretraining* on small-scale data. This enables contrastive self-supervised pretraining similar to methods used for large-scale models like SIMCLR or GPT-3. However, we only use small-scale 'task-internal' data for pretraining, which requires orders of magnitude less data and compute than these large-scale, 'task-external' pretraining approaches. Most NLP models translate back and forth between discrete words and continuous token embeddings, often involving a softmax computation that is limited to predicting classes known at training time. To ease learning from small data, our *first core idea is that text input words $\boldsymbol{w}_i \in \boldsymbol{x}$ and labels $\boldsymbol{w}^{\circ}_{i,l}$ should be mapped into the same word representation space, i.e. drawn from a shared embedding look-up table E, to replace dense to sparse translations with embedding-to-embedding matching.* We thus replace learning instance labels y_i by their corpus-internally pretrained FastText or randomly initialised word embeddings $\boldsymbol{l}^{\circ}_i \in L$, while others (Pappas & Henderson, 2019) use text descriptions to form label embeddings as the vector average over description word embeddings. As a result, *pretraining word embeddings means pretraining (favourably initialising) label embeddings.* Unknown labels (words), in turn, can be inferred from FastText subword embeddings (Bojanowski et al., 2017).

As outlined visually, left to right in Fig. 1, learning multi-label classification then becomes a contrastive learning problem of *matching the word-sequence embedding $\boldsymbol{t}_i$* of text i ②, with its c label (word-sequence) embeddings $\boldsymbol{l}^{\circ}_i = \{\boldsymbol{l}^{\circ}_{i,1}, \dots \boldsymbol{l}^{\circ}_{i,c}\}$ ③, by feeding c text-vs-label combinations $[[\boldsymbol{t}_i, \boldsymbol{l}^{\circ}_{i,1}], \dots, [\boldsymbol{t}_i, \boldsymbol{l}^{\circ}_{i,c}]]$ ④ to a binary classifier M ⑤ for matching. This means that instead of predicting c classes at once, we predict a batch of c, single-class, binary classifications using binary cross entropy ⑥, where c needs not be constant across

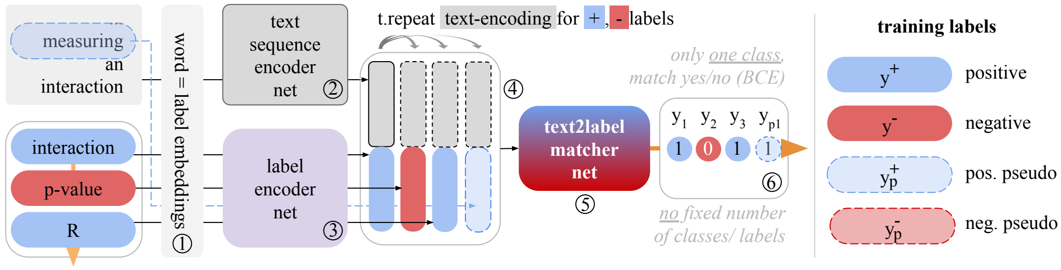

Figure 1: **Contrastive text-sequence-embedding-2-label-embedding matcher model:** A text ('measuring an interaction'), and positive ('interaction', R) or negative labels ('p-value') are encoded by the same word embedding layer E ①, where labels have word IDs for lookup. The text embeddings are then encoded by a sequence encoder T ②, while c labels are encoded by a label encoder L ③. Each text has multiple labels, so the text encoding $\boldsymbol{t}_i$ is repeated for, and concatenated with, each label encoding $\boldsymbol{l}^{\circ}_{i,l}$. The resulting batch of 'text-embedding, label-embedding' pairs $[[\boldsymbol{t}_i, \boldsymbol{l}^{\circ}_{i,1}], \ldots, [\boldsymbol{t}_i, \boldsymbol{l}^{\circ}_{i,c}]]$ ④ is fed into a 'matcher' classifier ⑤ that trains a binary cross entropy loss ⑥ on multiple label (mis-)matches $\{0, 1\}$ for each text instance $\boldsymbol{t}_i$. Words like 'measuring' provide self-supervised pseudo-labels. Positive and negative (pseudo-)labels are sampled from their own or other instances in a mini-batch.

instances i. The details of steps ① to ⑥ are as follows. To train a binary classifier, we need both positive and negative labels. Thus, for each text instance $\boldsymbol{w}_i = \{w_a, \ldots w_z\}$ we want to classify, we need g positive labels $\boldsymbol{w}_i^- = \{w_1^+, \ldots w_g^+\} \in R^g$ and b negative labels $\boldsymbol{w}_i^+ = \{w_1^-, \ldots w_b^-\} \in R^b$ to form a label selection vector $\boldsymbol{w}_i^{\circ} = \{\boldsymbol{w}^+ \oplus \boldsymbol{w}^-\} \in \mathbb{R}^{g+b}$. To indicate positive and negative labels, we also need a g sized vector of ones $\mathbf{1} \in \mathbb{R}^g$ and a b sized zero vector $\mathbf{0} \in \mathbb{R}^b$, to get a class indicator $\mathbb{I}_i = \{\mathbf{1} \oplus \mathbf{0}\} \in \mathbb{R}^{c=g+b}$. Both the text (word) indices $\boldsymbol{w}_i$ and the label indices $\boldsymbol{w}_i^{\circ}$ are passed through a shared 'word-or-label embedding' look-up-table E ①, after which they are passed through their respective encoder networks – T as text-sequence encoder, L as label encoder. Thus, the text-encoder produces a (single) text embedding vector $\boldsymbol{t}_i = T(E(\boldsymbol{w}_i))$ per text instance i ②. The label-encoder produces $c = g + n$ label embedding vectors $(\boldsymbol{l}_i^{\circ})$ that form a label-embedding matrix $\boldsymbol{L}_i = [\boldsymbol{l}_1^+, \ldots, \boldsymbol{l}_g^+, \boldsymbol{l}_1^-, \ldots, \boldsymbol{l}_b^-] \leftarrow L(E(\boldsymbol{w}_i^{\circ}))$ ③. As text-encoder T we use a (CNN→max-k-pooling→ReLU) sub-network, while the label-encoder L is simply an (average-pool) operation, since a single label $(\boldsymbol{w}_{i,j}^{\circ})$, e.g. 'multi'-'label', can consist of multiple words. To compare how similar the text-embedding $\boldsymbol{t}_i$ is to each label-embedding $\boldsymbol{l}_{i,j}^{\circ}$, we repeat $\boldsymbol{t}_i$ c times and combine text and label embeddings to get a text-vs-label-embedding matrix $\boldsymbol{M}_i = [[\boldsymbol{l}_{i,1}^+, \boldsymbol{t}_i], \ldots, [\boldsymbol{l}_{i,c}^-, \boldsymbol{t}_i]]$ ④ that is passed into the matcher network M ⑤ to produce a batch of c probabilities $\boldsymbol{p}_i = \{\sigma(M(\boldsymbol{M}_i)_1, \ldots, \sigma(M(\boldsymbol{M}_i)_c\}$ ⑥. As the optimisation loss, we the use binary cross entropy between $\boldsymbol{p}_i$ and $\mathbb{I}_i$, i.e. $\frac{1}{c}\sum_{l=1}^{c} \mathbb{I}_{i,l} \cdot log(\boldsymbol{p}_{i,l}) + (1 - \mathbb{I}_{i,l}) \cdot log(1 - \boldsymbol{p}_{i,l})$.

With label embeddings, a model can predict labels unseen at training time. Representations for such labels can be learned with self-supervision, using words as labels. This exploits both *transfer learning from inputs and labels*, using the matcher as a learned similarity function. Positive labels $\boldsymbol{w}_i^+$ can be supervision labels. Negative labels $\boldsymbol{w}_i^-$ can be sampled from the positive labels of other instances $\boldsymbol{w}_j^+$ in the same batch, *which avoids needing to know the label set beforehand*. Since *labels are words*, we can sample positive words from the current and negative words from other text instances to get pseudo-labels. *Sampling pseudo-labels provides a straight-forward contrastive, partial autoencoding mechanism usable as self-supervision in pretraining or as zero-shot learner*. Because both real and pseudo labels are sampled words, the model does not need to distinguish between them. Instead, learning is controlled by an out-of-model sampling routine for real supervision and pseudo self-supervision labels. This leads to a *second core idea: once inputs X and outputs Y are* *well initialised, the model Θ can also be better initialised by pretraining via self-supervision. As a result, we can learn supervised, few and zero-shot tasks in a unified manner.*

4 Long-tailed, noisy, text-to-text multi-label prediction

Since it is our goal to research *better few and zero-shot learning approaches for small pretraining models*, we choose a multi-label question tag prediction dataset as a testbed. We use the "Questions from Cross Validated"[1] dataset, where machine learning concepts are tagged per question. *There is currently no published baseline for this task.* The classes (tags) and input words are highly long-tailed (imbalanced). The first 20% of labels occur in only 7 'head' classes. Tags are highly sparse – at most 4 out of 1315 tags are labelled per question. Word embeddings are pretrained with FastText – details in appendix App. A.3. We use the labelled questions part of the dataset, which has 85k questions and 244k labels. What makes this problem particularly challenging is that 80% of the *least frequent labels* are distributed over 99.5% of classes, as an extreme long tail. The label density (% of active labels per question) is only 0.22% or $\approx 2.8/1305$ possible classes per instance. For a realistic evaluation setting, we split the dataset diachronically, using the 80% earliest documents for training, the next 10% for development, and the last 10% for testing.

Why not large external pretraining? Real-world, long-tailed datasets are thus always dominated by a low-learning-resource problem for most classes. This makes two things obvious: (A) that *model learning cannot simply be solved by using massive data sets as the long-tail problem grows as well*; (B) that *studying self-supervised pretraining on challenging, but smaller, long-tailed datasets such as this one, is useful for assessing a model's ability to learn from complex, real-world data.* We thus evaluate the effects of self-supervision in a noisy low-resource setup, also as a response to recent critiques of the evaluation metrics used to assess Web-scale learning (Linzen, 2020; Yogatama et al., 2019). As McCoy et al. (2019) shows, these evaluation setups are solvable by large-scale pattern overfitting, which, they find, leads to a 'Clever Hans effect', rather than real task progress.

5 Experimental setup and metrics

We want to analyse the *benefits of self-supervision for (a) fully supervised, (b) few and (c) zero-shot learning in a noisy low-resource, long-tailed, multi-label classification setting*. In this section, we describe suitable evaluation metrics, then discuss results in the next section.

Long-tail evaluation metrics and challenges: Long-tail, multi-label classification is challenging to evaluate. Many classification metrics are unsuitable for evaluating long-tailed datasets. They either: (i) misrepresent performance under class imbalance; (ii) do not scale to many classes; or (iii) are only meaningful if the desirable number of classes per instance is known (multi-label classification). For problem (i) ROC_{AUC} is known to overestimate imbalanced performance (Davis & Goadrich, 2006; Fernández et al., 2018), e.g. ROC_{AUC} test scores were upwards of .98 for most of our models. For problem (ii), measures such as F-score require discretisation threshold search for imbalanced prediction problems, i.e. searching for the optimal threshold per class (on a development set), which becomes computationally infeasible. Simply using a 0.5 probability threshold drives model selection towards balanced prediction, mismatching the long-tail problem. Metrics like precision@k handle problem (i-ii), but require knowledge of k, i.e. problem (iii): these metrics can only compare a chosen number of labels k, and cannot handle cases where the correct number of labels per instance varies or is unknown (label distribution shift). To more reliably measure performance under imbalance (i), to avoid unscalable class decision thresholding (ii), and to not optimise models for a set number of labels k per instance (iii), we use the average-precision (AP) score. It is defined as $AP = \sum_n (R_n - R_{n-1}) P_n$, where P_n and R_n are the precision and recall at the nth threshold. AP measures classifier performance over *all decision thresholds*, is computationally

[1] https://www.kaggle.com/stackoverflow/statsquestions

cheaper than threshold search, and allows for a dynamic number of labels per class. This latter property makes this task especially hard. A model has to learn when to predict a label, at what rarity, and how many such labels to predict for each instance. We also report the macro-averaged Brier-Score (BS) over all classes, as a scalable, compute-efficient measure of classifier calibration. Though more accurate measures exist, computing them is more involved and they require additional evaluation labour when optimising a specific supervised dataset, which is not our goal. For both measures, we use their popular scikit-learn implementations[2].

A challenging task, even for humans: On the dataset it is hard to guess how many labels per question to tag and how specific they should be, especially without domain knowledge. Out of the different weighting schemes for average precision, we choose AP_{micro} and AP_{macro}, as they are the most pessimistic (hardest to increase) measures to reduce optimistic evaluation. This choice is motivated by the goal of this work, which is to not simply to push end-task performance, but to use supervised learning scores as a proxy to evaluate the effects of pretraining on zero-shot learning as well as data-efficiency and speed of supervised and few-shot learning.

6 Results

In this section, we first analyse a normal and a strong supervised baseline to minimise overly favourable comparison against our subsequently evaluated self-supervision enhanced approaches. Finally, we analyse the benefits of 'dataset-internal' pretraining for few-shot learning, and how the amount of pretraining learning signal and model size affect zero-shot learning. *Test scores are reported according to the best dev set average precision score AP_{micro} over all classes.*

6.1 Baseline model results

In this section, we establish baseline results (**Base**) for a non-learning majority class baseline (ZeroR), a common ('weak') CNN baseline trained with binary-cross-entropy, and a solid CNN baseline optimised using a set of generalisation techniques proposed by Jiang et al. (2020). The **ZeroR** classifier is useful for establishing a baseline performance under class imbalance – e.g. if a class is present in only 10% of instances, then 90% accuracy is achieved by simply always predicting zero – i.e. the majority class. When doing so on our long-tailed task, where the class majority is always zero, we get an AP_{micro} and AP_{macro} of 0.2%, since out of the 1315 classes, maximally four classes are active per instance. Importantly, this tells us that: (a) simply learning to predict zeros can not score well on under this metric and (b) that this problem setting is challenging. Next, we evaluate both **a weak and optimised baselines (WB, OB).** When using a very small CNN as baseline (WB) with max pooling over 10 filters at filter sizes 1-3 that feed into a one-layer classifier, we achieved $33.75\% AP_{micro}$ on the test set – after only tuning the learning rate. When tuning this baseline for parameters known to increase generalisation using a set of such methods suggested by Jiang et al. (2020), we get a more solid test score of 45.01 AP_{micro} and an of 22.81 AP_{macro}. The macro result tells us that not all classes perform equally well. Upon closer inspection, we find that model performance worsens with increasing class rarity as expected. While establishing a solid baseline, we find expected limitations of model width, max-k pooling and dropout scale-up, and a confirmation that controlled experiment comparisons that only change one variable at a time, do not suffice to find better hyperparameter configurations. For example, when widening lower layer components and observing a decrease in performance, higher layers should also be made wider to accommodate the additional feature information from lower layers – which is consistent with findings in Nakkiran et al. (2020). A more detailed breakdown of this analysis can be found in Table Tab. 2 in the appendix App. A. We explore a considerable amount of hyperparameter configurations in an effort to compute a solid

[2] https://scikit-learn.org/stable/modules/model_evaluation.html

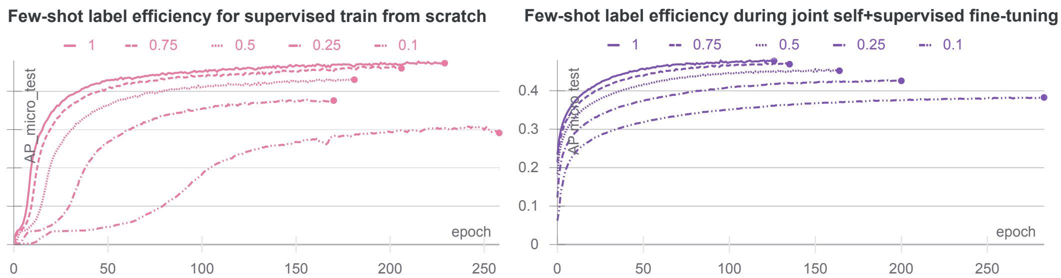

Figure 2: **Few-shot learning: Best training from scratch (left) vs. best fine-tuned (right)**: AP_{micro_test} curves for different few-shot portions: 100%, 75%, 50%, 25%, and 10% of training samples. *'Dataset-internal' pretraining via self-supervision (right) markedly improves few-shot learning performance, speed and stability* compared to training from scratch (left).

baseline. This allows for more robust insights and helps to speed up optimisation of the self-supervised models.

6.2 Full supervision (S(+S)Ls) as reference (*) for few and zero-shot learning

Tab. 1 show both: models trained From Scratch (s), and models that are first Pretrained (p) using self-supervised word pseudo-labels from text inputs, and afterwards fine-tuned (f) on supervision labels. To fit the supervised end-task (tag prediction), both fine-tuning and training from scratch can either: (1) only fit supervision labels (SL) or (2) jointly fit supervised labels and self-supervised word pseudo-labels (S(+S)L), as described in §3.

However, before analysing results, we define a controlled experiment setup using a fixed, but shared hyperparameter setting '(*) S(+S)Ls' as a reference (*). Since S(+S)Ls is the most basic model learning setup that uses both self-supervision and supervision, we use its optimal hyperparameters **'(*) S(+S)Ls'** as a fixed reference configuration for most subsequent learning setups, as indicated by the **'params like (*)'** marker. This ensures a more controlled comparison of the effects of pretraining vs. training from scratch, and robust insights on how to design self-supervision during end-task fitting and pretraining. **The (*) reference will hence be used for most few and zero-shot settings.** When comparing Pretrained models with models trained From Scratch, we see that *under comparable hyperparameters, without setting-specific parameter tuning, all four learning setups perform similarly* within 1 percent point (%p) of each other. We also see that the Pretrained model which uses self-supervision during both pretraining and fine-tuning performs best. Training From Scratch using self+supervision S(+S)Ls somewhat hurts performance compared to using supervision alone in SLs. Test scores are reported for the best dev set AP_{micro} scores.

6.3 Few-shot: pretrain for better long-tail, low-resource, few-shot learning

In this section, we present evidence that even in a data-limited, long-tailed setting, self-supervised *'data-internal'* pretraining: (a) increases few-shot learning performance of subsequent fine-tuning, while (b) improving learning speed and stability. This demonstrates that small data pretraining has similar benefits as large-scale pretraining (Brown et al., 2020; Schick & Schütze, 2020a). In Fig. 2, when using the (*) reference model from Tab. 1, we now compare training from scratch as before (pretraining off, left), with pretraining via self-supervised word pseudo-labels, and then fine-tuning on the supervised training labels of

Table 1: **Supervised long-tail prediction results:** comparing an optimized baseline (OB) with contrastive methods. Contrastive methods compare training from scratch vs. pretraining+fine-tuning vs. pretraining for few and zero-shot learning. Using the same hyperparameters (*) in a controlled experiment, the contrastive training results for the supervised end-task are all similar, but there are *fundamental performance differences as a result of self-supervised, contrastive pretraining when applied to the few and zero-shot learning settings* – details described in the subsections below.

Training method/ model	**learning setup**	**AP micro/ macro test %**	**Brier score macro**
Base: *baselines*			
ZeroR	always predict majority per class (=all zero)	00.20/00.20	n.a.
WB: weak baseline (BCE)	supervised	33.75/n.a.	n.a.
OB: optimized baseline (BCE)	supervised	45.01/22.81	0.0015
From Scratch: *supervised (SL), or self+supervised (S(+S)L) train from scratch (s) – no pretraining*			
(*) S(+S)Ls: h-params base	self+supervised scratch	47.13/25.28	0.0028
SLs: h-parms like (*)	supervised scratch	47.74/26.05	0.0028
Pretrained: *self-supervised (SSL) pretrain (p), then fine-tune (f)*			
S(+S)Lpf: h-parms like (*)	self pretrain >self+supervised fine-tune	48.20/25.58	0.0027
SLpf: h-parms like (*)	self pretrain >supervised fine-tune	47.53/25.65	0.0028
Few-Shot: *few-shot 10% train, 'pretrained then fine-tuned' (pf) vs from scratch (s)*			
SLpf: h-parms like (*)	self pretrain >10% supervised fine-tune	38.01/18.31	0.0037
S(+S)Lpf: h-parms like (*)	self pretrain >10% self+supervised fine-tune	38.25/18.49	0.0038
SLs: h-parms like (*)	10% supervised from scratch	30.46/13.07	0.0032
(*) S(+S)Ls:	10% self+supervised from scratch	30.53/13.28	0.0039
Zero-Shot: *zero-shot, self-supervised pretrain only*			
SSLp: h-parms, like (*)	self pretrain >zero-shot	10.26/10.70	0.1139
SSLp: extra h-param tuning	self pretrain >zero-shot	14.94/14.86	0.0791

the end-task (pretraining on). Note that our model architecture (Fig. 1) does not distinguish between self-supervised and supervised labels, which means that during self-supervised pretraining, we sample as many word pseudo-labels as real labels during supervised fine-tuning (or when supervising from scratch).

When fine-tuning the pretrained model on an increasingly difficult Few-Shot portion of (100%), 75%, 50%, 25% and only 10% of the supervised training data, we see large $AP_{micro|macro\_test}$ performance improvements compared to training From Scratch in both Tab. 1 and Fig. 2. On the right, in Fig. 2, we see that the pretrained models start with a higher epoch-0 performance, train faster, are more stable and achieve a markedly better few-shot end performance than the left-hand 'from scratch' setting. This is confirmed by detailed results for the 10% Few-shot setting in Tab. 1, where pretrained models (SLpf, S(+S)Lpf) achieve $\approx .38/.18 AP_{micro|macro\_test}$ compared to only $\approx .30/.13 AP_{micro|macro\_test}$ for models trained from scratch (see SLs or S(+S)Ls). This means that, *when using only 10% supervised labels, pretrained models still retain* 38.25/48.20*, or roughly* 80%*, of their fully supervised performance.* This provides evidence to answer the underlying question: "Do we really need more data for pretraining or can we simply increase self-supervision?". Very recent work by Bansal et al. (2020) has investigated this question for large-scale, self-supervised pretraining, where they showed that increasing self-supervision to create "a richer learning signal" benefits few-shot performance of large models. *Our results demonstrate that this is also the case for small-scale, non-Transformer pretrained models, even under a much more challenging long-tailed learning setting* than Bansal et al. (2020) examined. However, to better understand the benefits of using more self-supervised training signals and its relation

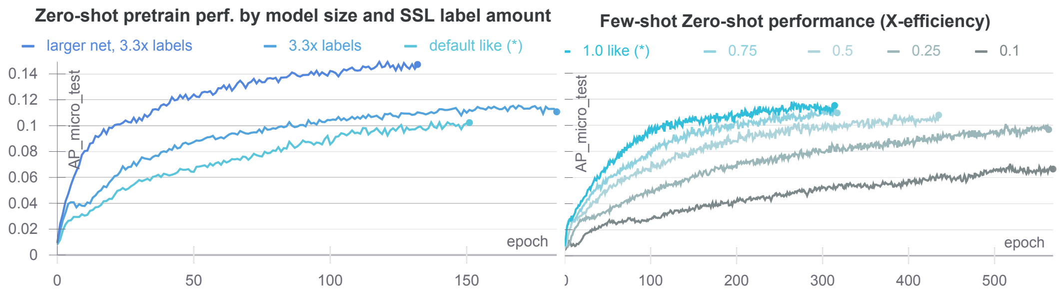

Figure 3: **Zero-shot performance by model and signal size: Left plot:** When using the same label and parameter amount as for the 'joint self+supervised train from scratch' reference model (*), allowing more self-supervision labels (left middle curve) and widening the network (left top curve) noticeably boosts zero-shot performance (supervised $AP_{micro\_dev\ and\ test}$). **Right:** when using less training data text (few-shot on inputs X), zero-shot still works, but we need to *wait much longer*.

to model size, we examine the zero-shot performance of our pretraining approach in regards to *label (signal) amount, network width and zero-shot X data-efficiency* (low-resource zero-shot performance) – i.e. zero-shot performance when pretraining on fractions of inputs X to forcibly limit self-supervision.

6.4 Zero-shot: more is better, for 'low-resource' zero-shot pretrain longer

In this experiment, we study how the number of self-supervised labels (signal) and the model width used for self-supervised pretraining affects zero-shot performance on the end-task test set. We show results in both Fig. 2 and Tab. 1 (ZERO-SHOT). In Fig. 2, we see that when using the reference hyperparameter configuration ((*) in Tab. 1), pretraining gets the lowest zero-shot performance. When increasing the number of self-supervised word pseudo-labels from 150 to 500, the model performs better (middle curve), while not using more parameters – so *increasing self-supervision signals is beneficial*. When additionally tripling the network's sequence and label encoder width and doubling the label match classifier size, zero-shot performance increases even more (top curve). This indicates that *for zero-shot learning performance from pretraining, both the amount of training signals and model size have a significant impact*. While increased model size has been linked to increased zero-shot performance of Web-scale pretrained models like GPT-3 (Brown et al., 2020), the influence of signal amount on zero-shot learning is much less well understood, because large-scale pretraining research often increases training data size when changing self-supervision, as outlined by Liu et al. (2020). Finally, in Fig. 3 we see that when pretraining our model for zero-shot prediction on only portions (100%, 75%, .50%, 25% and 10%) of the training text inputs X, i.e. an increasingly low-resource zero-shot setting, we still converge towards comparable full zero-shot performance (if we had not stopped early). However, each reduction in training size multiplies the required training time – when using the same number of self-labels. *This provides a promising insight into self-supervised pretraining on small datasets, which, if designed appropriately, can be used to pretrain well-initialised models for supervised fine-tuning and few-shot learning from very small text sizes.*

7 Conclusion

We showed that label-embedding prediction, modified for self-supervised pretraining on a challenging long-tail, low-resource dataset substantially improves low-resource few and zero-shot performance. We find that increased self-supervision, in place of increased data size or resorting to large-scale pretraining, strongly boosts few and zero-shot performance, even in challenging settings. In future, we envision that the proposed methods could be applied in scenarios where little in-domain (pre-)training data is available, e.g. in medicine (Şerbetci et al., 2020), and where new labels rapidly emerge at test time, e.g. for hashtag prediction (Ma et al., 2014). The code and data splits will be published on `https://github.com`.

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A Appendix

A.1 A baseline tuned using generalisation techniques

Table 2: **Building an optimised supervised baseline:** using test set generalization techniques as proposed by Jiang et al. (2020). %p denotes absolute percent points. Since parameters cannot be tuned in isolation, %p only reflects drops by deviating from optimal settings once they are found. Details on the explored hyperparameters are found in Tab. 3.

Model	**variable**	**observation**	**optimal parameter, %p drop from not using it**
pre-opt NN	learning rate optimized	base setting	33.75%p AP_{micro_test}
optimized NN	Optimal parameters ↓	base setting	45.01%p AP_{micro_test}, .0015 BS_{macro}
larger NN	max-k pooling	important	max-3 pooling, 3%p better than max-1 pooling
	CNN filter size	important	n-gram filter sizes >2 matter (∼2%p), comparing same filter amounts
	num CNN filters	important	100 filters per n-gram size
	wider classifier	overfitting	more than a 1 layer classifier lead to overfitting
dropout	on CNN output	improvement	2% better AP_{micro_test} test, 2%p improvement
	on deeper/ wider clf	none, stability	stabilizes learning, but same performance
optimizer	ADABOUND	failed	-39%p drop AP_{micro_test}, despite tuning
learning rate	lower LR	crucial	LR = 0.0075 for ADAM with cross-entropy
batch size	batch size	important	batch_size = 1024 worked well

For the baseline we found optimal hyperparameters to be: lr=0.0075, filter-sizes={1: 57, 2: 29, 3: 14}, clf=one_layer_classifier, 'conf':[{'do':.2}] , max-k pooling=3, bs=1536, tune embedding=True, optimizer=ADAM with pytorch defaults. Increasing the filter size, classifier size or depth or using more k decreased dev set performance due to increased overfitting. In general the standard multi-label BCE loss overfit much more quickly than the contrastive methods discribed in §3. The contrastive model only differs it was able to use more filters {1: 100, 2: 100, 3: 100}, where using only {1: 20, 2: 20, 3: 20} loses 1.5

Table 3: **Parameters we explored for the optimized baseline**. Not all combinations were tried. We tuned in order: learning rate lr, filter sizes, max-k pooling, tuning embeddings, batch size, classifier depth and lastly tried another optimizer.

Filters	{1: 57, 2: 29, 3: 14}, {1: 57, 2: 29, 10: 14},{1: 285, 2: 145, 3: 70}, {1:10, 10:10, 1:10}, {1:15, 2:10, 3:5}, {1:10}, {1:100}, {10:100}
Filter sizes	1, 2, 3, 10
lr	0.01, 0.0075, 0.005, 0.001, 0.0005, 0.0001
bs	1536, 4096
max-k	1, 3, 7
classifier	two_layer_classifier, 'conf':[{'do': None|.2, 'out_dim': 2048 | 4196 | 1024}, {'do':None| 0.2}]}, one_layer_classifier, 'conf':[{'do':.2}]}
tune embedding:	True, False
optimizer:	ADAM, ADABOUND by Luo et al. (2019) (very low results)

%p of performance, and that its optimal lr = 0.0005, while the batch size shrinks to 1024 due to increased memory requirements of label matching. This contrastive models optimal matcher classifier is deeper, due to the increased task complexity – four_layer_classifier, 'conf': [{'do': 0.2}, {'out_dim': 1024, 'do': 0.1}, {'out_dim': 300, 'do': None}, {'out_dim': 1, 'do': None}]}.

A.2 Few-shot: scratch, pretrained, additional self+supervised scenarios

Figure 4: **Few-shot training from scratch (top 2) vs. after pretraining (bottom 2)**: and using only supervision to fit the end-task (left) vs. jointly using self+supervision (right). Results are in AP_{micro_test} for different few-shot training set portions (1, 75%, 50%, 25%, 10%). Insight 1: self-supervision during end-task fitting makes no learning difference – i.e. when comparing top (or bottom) left (supervised) vsřight (self+supervised) sub-figures, they look nearly the same. Insight 2: *Pretraining (bottom figs.) via self-supervision markedly improves few-shot learning performance, speed and stability*, independent of fine-tuning via supervision (left) or self+supervised (right).

Few-shot challenges: Few-shot learning increases the long-tail problem. For 10% few shot learning, we train on 6800 instances, so many classes will be unseen at training time We will publish both the parsed data splits and a cleaned code version on Github to encourage experimenting with and extending to other low-resource 'text-to-text' self-supervision methods, additional evaluation metrics and datasets.

Few-shot, with and without self-supervision – as pretraining or for joint self+supervised fine tuning: Fig. 4 shows in more detail that the pretrained model (bottom) learns better, and that joint self+supervised end-task training (scratch or fine-tuned) makes no difference.

A.3 Text preprocessing details

We decompose tags such as 'p-value' as 'p' and 'value' and split latex equations into command words, as they would otherwise create many long, unique tokens. 10 tag words are not in the input vocabulary and thus we randomly initialise their embeddings. Though we never used this information, we parsed the text and title and annotated them with 'html-like' title, paragraph and sentence delimiters. The dataset is ordered and annotated by time. Dev and test set are therefore future data compared to the training data, which results in a non-stationary problem, though we never determined to what extend.