

---

# Fast Multi-Resolution Transformer Fine-tuning for Extreme Multi-label Text Classification

---

**Jiong Zhang**  
Amazon  
jiongz@amazon.com

**Wei-cheng Chang**  
Amazon  
chanweic@amazon.com

**Hsiang-fu Yu**  
Amazon  
rofu.yu@gmail.com

**Inderjit S. Dhillon**  
UT Austin & Amazon  
inderjit@cs.utexas.edu

## Abstract

Extreme multi-label text classification (XMC) seeks to find relevant labels from an extreme large label collection for a given text input. Many real-world applications can be formulated as XMC problems, such as recommendation systems, document tagging and semantic search. Recently, transformer based XMC methods, such as X-Transformer and LightXML, have shown significant improvement over other XMC methods. Despite leveraging pre-trained transformer models for text representation, the fine-tuning procedure of transformer models on large label space still has lengthy computational time even with powerful GPUs. In this paper, we propose a novel *recursive* approach, XR-Transformer to accelerate the procedure through recursively fine-tuning transformer models on a series of multi-resolution objectives related to the original XMC objective function. Empirical results show that XR-Transformer takes significantly less training time compared to other transformer-based XMC models while yielding better state-of-the-art results. In particular, on the public Amazon-3M dataset with 3 million labels, XR-Transformer is not only 20x faster than X-Transformer but also improves the Precision@1 from 51% to 54%. Our code is publicly available at <https://github.com/amzn/pecos>

## 1 Introduction

Many real-world applications such as open-domain question answering [1, 2], e-commerce dynamic search advertising [3, 4], and semantic matching [5], can be formulated as an extreme multi-label text classification (XMC) problem: given a text input, predict relevant labels from an enormous label collection of size  $L$ . In these applications,  $L$  ranges from tens of thousands to millions, which makes it very challenging to design XMC models that are both accurate and efficient to train. Recent works such as Parabel [3], Bonsai [6], XR-Linear [7] and AttentionXML [8], exploit the correlations among the labels to generate label partitions or hierarchical label trees (HLTs) which can be used to shortlist candidate labels to be considered during training and inference. While these methods are scalable in terms of the size of the label collection, most of them rely only on statistical representations (such as bag-of-words) or pooling from pre-generated token embeddings (such as word2vec) to vectorize text inputs.

In light of the recent success of deep pretrained transformers models such as BERT [9], XLNet [10] and RoBERTa [11] in various NLP applications, X-Transformer [12] and LightXML [13] propose to fine-tune pre-trained transformer models on XMC tasks to obtain new state-of-the-art results over the aforementioned approaches. Although transformers are able to better capture semantic meaning of textual inputs than statistical representations, text truncation is often needed in practice to reduce GPU memory footprint and maintain model efficiency. For example, X-Transformer truncates input texts

to contain the first 128 tokens before feeding it into transformer models. Efficiency of transformer fine-tuning poses another challenge for XMC applications. Directly fine-tuning transformer models on the original XMC task with a very large label collection is infeasible as both the training time and the memory consumption are linear in  $L$ . In order to alleviate this, both X-Transformer and LightXML adopt a similar approach to group  $L$  labels into  $K$  clusters of roughly equal size denoted by  $B$  and fine-tune transformers on the task to identify relevant label clusters (instead of labels themselves). If  $B \approx \sqrt{L}$  and  $K \approx \sqrt{L}$ , then both the training time and the memory requirement of the fine-tuning can be reduced to  $O(\sqrt{L})$  from  $O(L)$ . However, as pointed out in [8], the model performance would deteriorate due to the information loss from label aggregation. Thus, both X-Transformer and LightXML still choose a small constant  $B$  ( $\leq 100$ ) as the size of the label clusters. As a result, transformers are still fine-tuned on a task with around  $L/100$  clusters, which leads to a much longer training time compared with non-transformer based models. For example, it takes X-Transformer 23 and 25 days respectively to train on Amazon-3M and Wiki-500K even with 8 Nvidia V100 GPUs.

To address these issues, we propose XR-Transformer, an XMC architecture that leverages pre-trained transformer models and has much smaller training cost compared to other transformer-based XMC methods. Motivated by the multi-resolution learning in image generation [14-16] and curriculum learning [17], we formulate the XMC problem as a series of sub-problems with multi-resolution label signals and recursively fine-tune the pre-trained transformer on the coarse-to-fine objectives. In this paper, our contributions are as follows:

- We propose XR-Transformer, a transformer based framework for extreme multi-label text classification where the pre-trained transformer is recursively fine-tuned on a series of easy-to-hard training objectives defined by a hierarchical label tree. This allows the transformers to be quickly fine-tuned for a XMC problem with a very large number label collection progressively.
- To get better text representation and mitigate the information loss in text truncation for transformers, we take into account statistical text features in addition to the transformer text embeddings in our model. Also, a cost sensitive learning scheme by label aggregation is proposed to introduce richer information on the coarsified labels.
- We conduct experiments on 6 public XMC benchmarking datasets and our model takes significantly lower training time compared to other transformer-based XMC models to yield better state-of-the-art results. For example, we improve the state-of-the-art Prec@1 result on Amazon-3M established by X-Transformer from 51.20% to 54.04% while reducing the required training time from 23 days to 29 hours using the same hardware.

## 2 Related Works

**Sparse Linear Models with Partitioning Techniques.** Conventional XMC methods consider fixed input representations such as sparse TF-IDF features and study different partitioning techniques or surrogate loss functions on the large output spaces to reduce complexity. For example, sparse linear one-versus-all (OVA) methods such as DiSMEC [18], PPD-Sparse [19, 20], ProXML [21] explore parallelism to solve OVA losses and reduce the model size by weight truncations.

The inference time complexity of OVA models is linear in the output space, which can be greatly improved by partitioning methods or approximate nearest neighbor (ANN) indexing on the label spaces. Initial works on tree-based methods [22, 23] reduce the OVA problem to one-versus-some (OVS) with logarithmic depth trees. Down that path, recent works on sparse linear models including Parabel [3], eXtremeText [24], Bonsai [6], XReg [25], NAPKINXC [26, 27] and XR-Linear [7] partition labels with  $B$ -array hierarchical label trees (HLT), leading to inference time complexity that is logarithmic in the output space. On the other hand, low-dimensional embedding-based models often leverage ANN methods to speed up the inference procedure. For example, AnnexML [28] and SLICE [29] consider graph-based methods such as HNSW [30] while GLaS [31] considers product quantization variants such as ScaNN [32].

**Shallow Embedding-based Methods.** Neural-based XMC models employ various network architectures to learn semantic embeddings of the input text. XML-CNN [33] applies one-dimensional CNN on the input sequence and use the BCE loss without sampling, which is not scalable to XMC problems. AttentionXML [8] employs BiLSTMs and label-aware attention as scoring functions. For better scalability to large output spaces, only a small number of positive and hard negative labels

are used in model GPU training. Shallow embedding-based methods [34-38] use word embedding lookup followed by shallow MLP layers to obtain input embeddings. For instance, MACH [34] learns MLP layers on several smaller XMC sub-problems induced by hashing tricks on the large label space. Similarly, DeepXML [35] and its variant (i.e., DECAF [36], GalaXC [37], ECLARE [38]) pre-train MLP encoders on XMC sub-problems induced by label clusters. They freeze the pre-trained word embedding and learn another MLP layer followed by a linear ranker with sampled hard negative labels from HNSW [30]. Importantly, shallow embedding-based methods only show competitive performance on short-text XMC problems where the number of input tokens is small [34-35].

**Deep Transformer Models.** Recently, pre-trained Transformer models [9-11] have been applied to XMC problems with promising results [12-13-39]. X-Transformer [12] considers a two-stage approach where the first stage transformer-based encoders are learned on XMC sub-problems induced by balanced label clusters, and the second stage sparse TF-IDF is combined with the learned neural embeddings as the input to linear OVA models. APLC-XLNet [39] fine-tunes XLNet encoder on adaptive imbalanced label clusters based on label frequency similar to Adaptive Softmax [40]. LightXML [13] fine-tunes Transformer encoders with the OVA loss function end-to-end via dynamic negative sampling from the matching network trained on label cluster signals. Nonetheless, Transformer-based XMC models have larger model size and require longer training time, which hinders its practical usage on different downstream XMC problems.

### 3 Background Material

We assume we are given a training set  $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^N$  where  $\mathbf{x}_i \in \mathcal{D}$  is the  $i$ th input document and  $\mathbf{y}_i \in \{0, 1\}^L$  is the one hot label vector with  $y_{i,\ell} = 1$  indicating that label  $\ell$  is relevant to instance  $i$ . The goal of eXtreme Multi-label Text Classification (XMC) is to learn a function  $f : \mathcal{D} \times [L] \mapsto \mathbb{R}$ , such that  $f(\mathbf{x}, \ell)$  denotes the relevance between the input  $\mathbf{x}$  and the label  $\ell$ . In practice, labels with the largest  $k$  values are retrieved as the predicted relevant labels for a given input  $\mathbf{x}$ . The most straightforward model is one-versus-all (OVA) model:

$$f(\mathbf{x}, \ell) = \mathbf{w}_\ell^\top \Phi(\mathbf{x}); \ell \in [L], \quad (1)$$

where  $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_L] \in \mathbb{R}^{d \times L}$  are the weight vectors and  $\Phi : \mathcal{D} \mapsto \mathbb{R}^d$  is the text vectorizer that maps  $\mathbf{x}$  to  $d$ -dimensional feature vector.  $\Phi(\cdot)$  could be a deterministic text vectorizer, such as the bag-of-words (BOW) model or Term Frequency-Inverse Document Frequency (TFIDF) model, or a vectorizer with learnable parameters. With the recent development in deep learning, using pre-trained transformer as the text vectorizer has shown promising results in many XMC applications [12-13-39]. When  $L$  is large, however, training and inference of OVA model without sampling would be prohibitive due to the  $O(L)$  time complexity.

To handle the extremely large output space, recent approaches partition the label space to shortlist the labels considered during training and inference. In particular, [7-12-13-34-35-39] follow a three stage framework: partitioning, shortlisting, and ranking. First, label features are constructed to group labels into  $K$  clusters  $\mathbf{C} \in \{0, 1\}^{L \times K}$  where  $C_{\ell,k} = 1$  denotes that label  $\ell$  is included in the  $k$ -th cluster. Then a shortlisting model is learned to match input  $\mathbf{x}$  to relevant clusters in an OVA setting:

$$g(\mathbf{x}, k) = \hat{\mathbf{w}}_k^\top \Phi_g(\mathbf{x}); k \in [K]. \quad (2)$$

Finally, a classification model with output size  $L$  is trained on the shortlisted labels:

$$f(\mathbf{x}, \ell) = \mathbf{w}_\ell^\top \Phi(\mathbf{x}); \ell \in S_g(\mathbf{x}), \quad (3)$$

where  $S_g(\mathbf{x}) \subset [L]$  is the label set shortlisted by  $g(\mathbf{x}, \cdot)$ . In the extreme case where only one label cluster is determined to be relevant to a input  $\mathbf{x}$ , the training and inference cost on  $\mathbf{x}$  would be  $O(K + \frac{L}{K})$ , which in the best case scenario is  $O(\sqrt{L})$  when  $K = \sqrt{L}$ .

For transformer based methods, the dominant time is the evaluation of  $\Phi(\mathbf{x})$ . But  $K$  being too big or too small could still be problematic. Empirical results show that the model performance deteriorates when clusters are too big [8]. This is because that the signals coming from  $B$  labels within the same cluster will be aggregated and not distinguishable, where  $B$  is the cluster size. Therefore,  $B$  cannot be too big to ensure a reasonable label resolution for fine-tuning. Also, as pointed out in [12], fine-tuning transformer models on large output spaces can be prohibitive. As a result, the label clusters need to

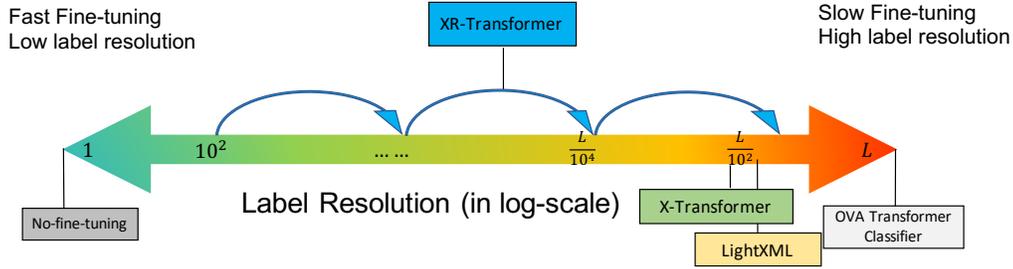


Figure 1: Illustration of fine-tuning on XMC tasks of different label resolutions. For an XMC task with a low label resolution, fine-tuning can be fast but model performance might deteriorate due to large deviation from the original XMC task. In practice, X-Transformer and LightXML adopt a XMC task with a relatively higher label resolution to ensure reasonable model performance at the cost of longer training time. The proposed XR-Transformer leverages multi-resolution learning and model bootstrapping that achieves both fast fine-tuning and good model performance.

be constructed in a way to balance the model performance and fine-tuning efficiency. In practice, both the transformer-based XMC models, such as X-Transformer and LightXML, adopt a small fixed constant as the cluster size  $B (\leq 100)$ , which means that training the shortlisting model  $g(\mathbf{x}, k)$  is still very time consuming as the number of clusters  $K \approx L/B$ .

#### 4 Proposed Method: XR-Transformer

As noted above, the shortlisting problem (2) is itself an XMC problem with slightly smaller output size  $\frac{L}{B}$  where  $B$  is the cluster size. In XR-Transformer, we apply the same three stage framework recursively on the shortlisting problem until a reasonably small output size is reached  $\frac{L}{B^D}$ . We can therefore follow the curriculum learning scheme and fine-tune the pre-trained transformers progressively on the sub-XMC problems with increasing output space  $\{\frac{L}{B^D}, \frac{L}{B^{D-1}}, \dots\}$ . At each fine-tuning task, the candidate label set is shortlisted by the final model at the previous task. The recursive shortlisting ensures that for any input, the number of candidate labels to include in training and inference is  $O(B)$  and therefore the total number of considered labels is  $O(B \log_B(L))$ . Also, we leverage the multi-step fine-tuning and use the embedding generated at the previous task to bootstrap the non pre-trained part for the current task. We now describe the model design in detail.

**Hierarchical Label Tree (HLT).** Recursively generating label clusters  $D$  times is equivalent to building a HLT [41] of depth  $D$ . We first construct label features  $\mathbf{Z} \in \mathbb{R}^{L \times \hat{d}}$ . This could be done by applying text vectorizers on label text or from Positive Instance Feature Aggregation (PIFA):

$$\mathbf{Z}_\ell = \frac{\mathbf{v}_\ell}{\|\mathbf{v}_\ell\|}; \text{ where } \mathbf{v}_\ell = \sum_{i: y_{i,\ell}=1} \Phi(\mathbf{x}_i), \forall \ell \in [L], \quad (4)$$

where  $\Phi : \mathcal{D} \mapsto \mathbb{R}^{\hat{d}}$  is the text vectorizer. Then we follow similar procedures as [8] and [13] and use balanced k-means ( $k = B$ ) to recursively partition label sets and generate the HLT in a top-down fashion. The HLT is represented with a series of indexing matrices  $\{\mathbf{C}^{(t)}\}_{t=1}^D$ , such that  $\mathbf{C}^{(t)} \in \{0, 1\}^{K_t \times K_{t-1}}$  where  $K_0 = 1$  and  $K_D = L$ . Equivalently, once  $\mathbf{C}^{(D)}$  is constructed, the HLT can be built from bottom up through joining  $B$  adjacent clusters together.

**Multi-resolution Output Space.** Multi-resolution learning has been explored in different contexts such as computer vision [14, 42]. For instance, using an output scheme with coarse-to-fine resolutions results in better image quality for generative adversarial networks [15, 16]. As another example in meta learning, [43] learns multiclass models via auxiliary meta classes by collapsing existing classes. Nevertheless, multi-resolution learning has not been well-explored in the XMC literature. In XR-Transformer, we leverage the label hierarchy defined by the HLT and train the transformer model on multi-resolution objectives.

The XMC task can be viewed as generating an 1-D image  $\mathbf{y} \in \{0, 1\}^L$  with binary values based on input text  $\mathbf{x}$ . Just like a coarsified image could be obtained by a max or mean pooling of nearby pixels,

the coarse label vector can be obtained by max-pooling of labels which are nearby in the label feature space. Once the HLT is constructed using label features, the true labels at layer  $\mathbf{Y}^{(t)} \in \{0, 1\}^{N \times K_t}$  can be determined by the true labels of the child clusters at  $t + 1$  through a max-pooling like operation:

$$\mathbf{Y}^{(t)} = \text{binarize}(\mathbf{Y}^{(t+1)} \mathbf{C}^{(t+1)}), \quad (5)$$

and  $Y_{i,\ell}^{(D)} = y_{i,\ell}$  is the original label matrix. This forms a series of learning signals with coarse-to-fine resolution and can be used to generate learning tasks with easy-to-hard objectives.

Direct use of the binarized  $\mathbf{Y}^{(t)} \in \{0, 1\}^{N \times K_t}$  in Eq (5) results in information loss when merging several positive labels into one cluster. Ideally, a cluster containing several positive children is more relevant than a cluster with only one positive child. To add this lower level information to higher level learning objectives, we introduce the relevance matrix  $\mathbf{R}^{(t)} \in \mathbb{R}_+^{N \times K_t}$  for layer  $t$  of the XMC sub-problem where  $R_{i,\ell}$  defines the non-negative important weight for  $i$ th instance to  $\ell$ th cluster. Different from cost-sensitive learning [44] for MLC (CSMLC) setting [45-47] where there is only one cost matrix explicitly derived by evaluation metrics such as F1 score, in XR-Transformer, we consider the usage of cost-sensitive learning where the relevance matrices are recursively induced by the HLT structure. Specifically, given an HLT, we recursively construct relevance matrices for  $t = 1, \dots, D$ :

$$\mathbf{R}^{(t)} = \mathbf{R}^{(t+1)} \mathbf{C}^{(t+1)}, \quad (6)$$

and  $\mathbf{R}^{(D)} = \mathbf{Y}^{(D)}$ . Motivated by [48], we adopt the row-wise  $\ell_1$  normalized relevance matrix:

$$\hat{R}_{i,j}^{(t)} = \begin{cases} \frac{R_{i,j}^{(t)}}{\|\mathbf{R}_i^{(t)}\|_1} & \text{if } Y_{i,j}^{(t)} = 1, \\ \alpha & \text{otherwise,} \end{cases}$$

where  $\alpha$  is the hyper parameter to balance positive and negative weights.

**Label Shortlisting.** During training, XR-Transformer only focuses on discriminating the labels or clusters that have high chance of being positive. A necessary condition for a label at layer  $t$  to be positive is that its parent label at level  $t - 1$  is positive. Therefore, an intuitive approach would be to only train on the output space shortlisted by positive clusters of the parent layer. However, in practice we found this approach sometimes leads to sub-optimal result during inference with beam search. As an effort to balance explore and exploit, we further include the top- $k$  relevant clusters determined by the model learned on the parent layer to mimic the beam search during inference. Thus at layer  $t$ , the labels considered during training are shortlisted by the parent layer  $t - 1$ :

$$\mathbf{P}^{(t-1)} = \text{Top}(\mathbf{W}^{(t-1)\top} \Phi(\mathbf{X}, \Theta^{(t-1)}), k), \quad (7)$$

$$\mathbf{M}^{(t)} = \text{binarize}(\mathbf{P}^{(t-1)} \mathbf{C}^{(t)\top}) + \text{binarize}(\mathbf{Y}^{(t-1)} \mathbf{C}^{(t)\top}), \quad (8)$$

where the  $\text{Top}(\cdot, k)$  operator zeros out elements in a matrix except the top- $k$  largest values in each row. For each instance  $\mathbf{x}_i$ , only non-zero indices of  $\mathbf{M}_i$  will be included into the training objective. We can therefore define a series of learning objectives for level  $t \in \{1, 2, \dots, D\}$  as:

$$\min_{\mathbf{W}^{(t)}, \Theta} \sum_{i=1}^N \sum_{\ell: \mathbf{M}_{i,\ell}^{(t)} \neq 0} \hat{R}_{i,\ell}^{(t)} \mathcal{L}(Y_{i,\ell}^{(t)}, \mathbf{W}_\ell^{(t)\top} \Phi(\mathbf{x}_i, \Theta)) + \lambda \|\mathbf{W}^{(t)}\|^2, \quad (9)$$

where  $\mathcal{L}$  is a point-wise loss such as hinge loss, squared hinge loss or BCE loss,  $\mathbf{W}^{(t)}$ ,  $\Theta$  are the model weights to be learned.

**Text Representation.** Most previous works on XMC construct text feature representation in one of two ways: statistical feature representations and semantic feature representations. Although the latter, in particular transformer models, have shown promising results on various NLP benchmarks, the self-attention mechanism makes transformers unscalable w.r.t. sequence length. To ensure efficiency, input texts are usually truncated [12, 13] which result in loss of information. On the other hand, the statistical features, such as TFIDF, are fast to construct with the whole input taken into consideration. In XR-Transformer, we use a combination of these two feature representations and each component is a complement of lost information for the other one:

$$\Phi_{cat}(\mathbf{x}, \Theta) := \left[ \frac{\Phi_{tfidf}(\mathbf{x})}{\|\Phi_{tfidf}(\mathbf{x})\|}, \frac{\Phi_{dnn}(\mathbf{x}, \Theta)}{\|\Phi_{dnn}(\mathbf{x}, \Theta)\|} \right], \quad (10)$$

---

**Algorithm 1:** Iterative\_Learn( $\mathbf{X}, \mathbf{Y}, \mathbf{C}, \theta, \mathbf{P}$ )

---

**Input** :  $\mathbf{X}, \mathbf{Y}, \mathbf{C}, \theta, \mathbf{P}$  $m, n \leftarrow \mathbf{C}.shape$ **if**  $n = 1$  **then**     $\mathbf{M} \leftarrow ones(N, m)$     **if**  $\theta$  is not fixed **then**         $\theta^* \leftarrow$  Optimize (9) with  $\Phi = \Phi_{dnn}$ , initialize  $\Theta = \theta$     **else**         $\theta^* \leftarrow \theta$      $\mathbf{W}^* \leftarrow \operatorname{argmin}_{\mathbf{W}} \sum_{i=1}^N \sum_{\ell=1}^m \hat{R}_{i,\ell}^{(t)} \mathcal{L}(Y_{i,\ell}, \mathbf{W}_{\ell}^{\top} \Phi_{cat}(\mathbf{x}_i, \Theta)) + \lambda \|\mathbf{W}\|^2$ **else**     $\mathbf{Y}_{prev} \leftarrow \operatorname{binarize}(\mathbf{Y}\mathbf{C})$      $\mathbf{M} \leftarrow \operatorname{binarize}(\mathbf{P}\mathbf{C}^{\top}) + \operatorname{binarize}(\mathbf{Y}_{prev}\mathbf{C}^{\top})$     **if**  $\theta$  is not fixed **then**         $\theta^* \leftarrow$  Optimize (9) with  $\Phi = \Phi_{dnn}$  initialize  $\Theta = \theta$     **else**         $\theta^* \leftarrow \theta$      $\mathbf{W}^* \leftarrow \operatorname{argmin}_{\mathbf{W}} \sum_{i=1}^N \sum_{\ell: \mathbf{M}_{i,\ell} \neq 0} \hat{R}_{i,\ell}^{(t)} \mathcal{L}(Y_{i,\ell}, \mathbf{W}_{\ell}^{\top} \Phi_{cat}(\mathbf{x}_i, \theta^*)) + \lambda \|\mathbf{W}\|^2$ **Return** :  $\mathbf{W}^*, \theta^*$ 

---

---

**Algorithm 2:** XR-Transformer training

---

**Input** :  $\mathbf{X}, \mathbf{Y}$ , pre-trained transformer  $\Phi_{dnn}(\cdot, \theta_0)$  $\hat{\mathbf{Z}}_{\ell} = \mathbf{v}_{\ell} / \|\mathbf{v}_{\ell}\|$ ; where  $\mathbf{v}_{\ell} = \sum_{i: y_{i,\ell}=1} \Phi_{tfidf}(\mathbf{x}_i), \forall \ell \in [L]$  $\{\hat{\mathbf{C}}^{(t)}\}_{t=1}^{\hat{D}} \leftarrow$  k-means-clustering( $\hat{\mathbf{Z}}$ )Generate label hierarchy  $\{\hat{\mathbf{Y}}^{(t)}\}_{t=1}^{\hat{D}}$  using 5 $\theta^* = \theta_0, \mathbf{P} = None$ **for**  $t$  in  $1, 2, 3, \dots, \hat{D}$  **do**     $\hat{\mathbf{W}}, \theta^* \leftarrow$  Iterative\_Learn( $\mathbf{X}, \hat{\mathbf{Y}}^{(t)}, \hat{\mathbf{C}}^{(t)}, \theta^*, \mathbf{P}$ )     $\mathbf{P} \leftarrow \operatorname{Top}(\hat{\mathbf{W}}^{\top} \Phi_{cat}(\mathbf{X}, \theta^*), k)$  $\mathbf{Z}_{\ell} = \mathbf{v}_{\ell} / \|\mathbf{v}_{\ell}\|$ ; where  $\mathbf{v}_{\ell} = \sum_{i: y_{i,\ell}=1} \Phi_{cat}(\mathbf{x}_i), \forall \ell \in [L]$  $\{\mathbf{C}^{(t)}\}_{t=1}^D \leftarrow$  k-means-clustering( $\mathbf{Z}$ )Generate label hierarchy  $\{\mathbf{Y}^{(t)}\}_{t=1}^D$  using 5Fix  $\theta^*, \mathbf{P} = None$ **for**  $t$  in  $1, 2, 3, \dots, D$  **do**     $\mathbf{W}^{(t)}, \_ \leftarrow$  Iterative\_Learn( $\mathbf{X}, \mathbf{Y}^{(t)}, \mathbf{C}^{(t)}, \theta^*, \mathbf{P}$ )     $\mathbf{P} \leftarrow \operatorname{Top}(\mathbf{W}^{(t)\top} \Phi_{cat}(\mathbf{X}, \theta^*), k)$ **Return** :  $\Phi_{cat}(\cdot, \theta^*), \{\mathbf{C}^{(t)}\}_{t=1}^D, \{\mathbf{W}^{(t)}\}_{t=1}^D$ 

---

where  $\Phi_{dnn}(\cdot, \Theta)$  is the transformer parametrized by  $\Theta$ . Once the text representation is constructed, predictions can be made by simply applying a linear projection on top of the text representation through (1).

**Training with bootstrapping.** The training of XR-Transformer consists of three steps. At first, a preliminary HLT is constructed using raw statistical features. Then a pre-trained transformer model is fine-tuned recursively from low resolution output to high resolution. At each layer  $t$ , fine-tuning objective (9) is optimized with initialization  $\Theta = \theta^{(t-1)*}$  the best transformer weights of layer  $t - 1$ .  $\theta^{(0)*}$  denotes the pre-trained transformer weights.

Unlike the transformer warmed-up with pre-trained weights, the projection weights  $\mathbf{W}^{(t)}$  is trained from scratch without good initialization. At the beginning of fine-tuning, gradient flow through these cold-start (usually randomly initialized) weights will usually worsen the pre-trained components.

We leverage the recursive learning structure to tackle this issue by model bootstrapping. Concretely,  $\mathbf{W}^{(t)}$  is initialized as:

$$\mathbf{W}_{init}^{(t)} := \operatorname{argmin}_{\mathbf{W}^{(t)}} \sum_{i=1}^N \sum_{\ell: \mathbf{M}_{i,\ell}^{(t)} \neq 0} \hat{R}_{i,\ell}^{(t)} \mathcal{L}(Y_{i,\ell}^{(t)}, \mathbf{W}_{\ell}^{(t)\top} \Phi_{dnn}(\mathbf{x}_i, \boldsymbol{\theta}^{(t-1)*})) + \lambda \|\mathbf{W}^{(t)}\|^2, \quad (11)$$

In practice, (11) is fast to compute since the semantic text feature for the previous layer  $\Phi_{cat}(\mathbf{X}, \boldsymbol{\theta}^{(t-1)*})$  is already computed and thus (11) can be solved very quickly on CPUs with a variety of parallel linear solvers, such as LIBLINEAR [49].

Once the fine-tuning is complete, the refined HLT is constructed with the text representation that combines statistical text feature and fine-tuned semantic text embeddings. Then the ranking models are trained on top of the combined text features for the final prediction. The detailed training procedure is described in Algorithm 1 and 2.

**Inference.** The inference cost of XR-Transformer consists mainly of two parts: cost to compute transformer embedding and to retrieve relevant labels through beam search. Therefore, the inference time complexity is  $O(T_{dnn} + kd \log(L))$ , where  $k$  is the beam size,  $d$  is the concatenated feature dimension and  $T_{dnn}$  is the time to compute  $\Phi_{dnn}(\mathbf{x})$  for a given input. Note that even the inference is done with beam search through the refined HLT, the transformer text embedding only need to be computed once per instance.

**Connections with other tree based methods.** Although methods such as AttentionXML [8] also train on supervisions induced by label trees, the final model is a chain of sub-models which each on is learned on single-resolution. In particular, given a hierarchical label tree with depth  $D$ , AttentionXML will train  $D$  different text encoders on each layer of the tree where as XR-Transformer trains the same transformer encoder progressively on all layers of the tree. This difference leads to a longer inference time for AttentionXML than XR-Transformer since multiple text encoders need to be queried during inference, as shown in the comparison in the inference time in Appendix A.4.2

## 5 Experimental Results

We evaluate XR-Transformer on 6 public XMC benchmarking datasets: Eurlex-4K, Wiki10-31K, AmazonCat-13K, Wiki-500K, Amazon-670K, Amazon-3M. Data statistics are given in Table 1. For fair comparison, we use the same raw text input, sparse feature representations and same train-test split as AttentionXML [8] and other latest works [12, 13]. The evaluation metric is Precision@k (P@k), which is widely-used in XMC literature [3, 8, 12, 13, 18, 28]. The results of Propensity-score Precision@k (PSP@k) are defer to Appendix A.4.3 which focus more on tail labels’ performance.

Table 1: Data statistics.  $N_{train}, N_{test}$  refer to the number of instances in the training and test sets, respectively.  $L$ : the number of labels.  $\bar{L}$ : the average number of positive labels per instance.  $\bar{n}$ : average number of instances per label.  $d_{tfidf}$ : the sparse feature dimension of  $\Phi_{tfidf}(\cdot)$ . These six publicly available benchmark datasets, including the sparse TF-IDF features are downloaded from <https://github.com/yourh/AttentionXML> which are the same as AttentionXML [8] X-Transformer [12] and LightXML [13] for fair comparison.

Dataset	$N_{train}$	$N_{test}$	$L$	$\bar{L}$	$\bar{n}$	$d_{tfidf}$
Eurlex-4K	15,449	3,865	3,956	5.30	20.79	186,104
Wiki10-31K	14,146	6,616	30,938	18.64	8.52	101,938
AmazonCat-13K	1,186,239	306,782	13,330	5.04	448.57	203,882
Wiki-500K	1,779,881	769,421	501,070	4.75	16.86	2,381,304
Amazon-670K	490,449	153,025	670,091	5.45	3.99	135,909
Amazon-3M	1,717,899	742,507	2,812,281	36.04	22.02	337,067

**Baseline Methods.** We compare XR-Transformer with state-of-the-art (SOTA) XMC methods: AnnexML [28], DiSMEC [18], PfastreXML [41], Parabel [3], eXtremeText [24], Bonsai [50], XML-CNN [33], XR-Linear [7], AttentionXML [8], X-Transformer [12] and LightXML [13]. We obtain

Table 2: Comparison of XR-Transformer with recent XMC methods on six public datasets. Results with a trailing reference are taken from [8] Table 3] and [7] Table 3]. We obtain the results of AttentionXML\*, LightXML\*, X-Transformer\* and XR-Transformer\* on the same vectorized feature matrix provided in [8]. Due to GPU memory constraint, LightXML is not able to run on Amazon-3M. The PSP@k results are available in Appendix A.4.3]

Methods	P@1	P@3	P@5	P@1	P@3	P@5	P@1	P@3	P@5
	Eurlex-4K			Wiki10-31K			AmazonCat-13K		
AnnexML [28]	79.66	64.94	53.52	86.46	74.28	64.20	93.54	78.36	63.30
DiSMEC [18]	83.21	70.39	58.73	84.13	74.72	65.94	93.81	79.08	64.06
PfastreXML [41]	73.14	60.16	50.54	83.57	68.61	59.10	91.75	77.97	63.68
Parabel [3]	82.12	68.91	57.89	84.19	72.46	63.37	93.02	79.14	64.51
eXtremeText [24]	79.17	66.80	56.09	83.66	73.28	64.51	92.50	78.12	63.51
Bonsai [50]	82.30	69.55	58.35	84.52	73.76	64.69	92.98	79.13	64.46
XML-CNN [33]	75.32	60.14	49.21	81.41	66.23	56.11	93.26	77.06	61.40
XR-Linear [7]	84.14	72.05	60.67	85.75	75.79	66.69	94.64	79.98	64.79
AttentionXML*	86.93	74.12	62.16	87.34	78.18	69.07	95.84	82.39	67.32
X-Transformer*	87.61	75.39	63.05	88.26	78.51	69.68	96.48	83.41	68.19
LightXML*	87.15	75.95	<b>63.45</b>	<b>89.67</b>	79.06	69.87	96.77	<b>83.98</b>	<b>68.63</b>
XR-Transformer*	<b>88.41</b>	<b>75.97</b>	63.18	88.69	<b>80.17</b>	<b>70.91</b>	<b>96.79</b>	83.66	68.04
	Wiki-500K			Amazon-670K			Amazon-3M		
AnnexML [28]	64.22	43.15	32.79	42.09	36.61	32.75	49.30	45.55	43.11
DiSMEC [18]	70.21	50.57	39.68	44.78	39.72	36.17	47.34	44.96	42.80
PfastreXML [41]	56.25	37.32	28.16	36.84	34.23	32.09	43.83	41.81	40.09
Parabel [3]	68.70	49.57	38.64	44.91	39.77	35.98	47.42	44.66	42.55
eXtremeText [24]	65.17	46.32	36.15	42.54	37.93	34.63	42.20	39.28	37.24
Bonsai [50]	69.26	49.80	38.83	45.58	40.39	36.60	48.45	45.65	43.49
XML-CNN [33]	-	-	-	33.41	30.00	27.42	-	-	-
XR-Linear [7]	65.59	46.72	36.46	43.38	38.40	34.77	47.40	44.15	41.87
AttentionXML*	76.74	58.18	45.95	47.68	42.70	38.99	50.86	48.00	45.82
X-Transformer*	77.09	57.51	45.28	48.07	42.96	39.12	51.20	47.81	45.07
LightXML*	77.89	58.98	45.71	49.32	44.17	40.25	-	-	-
XR-Transformer*	<b>79.40</b>	<b>59.02</b>	<b>46.25</b>	<b>50.11</b>	<b>44.56</b>	<b>40.64</b>	<b>54.20</b>	<b>50.81</b>	<b>48.26</b>

Table 3: Comparing training time (in hours) of DNN-based methods that produce the SOTA results in Table 2]. The number following the model indicates the number of ensemble models used.

Dataset	AttentionXML-3	X-Transformer-9	LightXML-3	XR-Transformer-3
Eurlex-4K		0.9	7.5	16.9
Wiki10-31K		<b>1.5</b>	14.1	26.9
AmazonCat-13K		24.3	147.6	310.6
Wiki-500K		<b>37.6</b>	557.1	271.3
Amazon-670K		24.2	514.8	159.0
Amazon-3M		54.8	542.0	-

most baseline results from [8] Table 3] and [7] Table 3] except for the latest deep learning based algorithms [8] [12] [13]. To have fair comparison on training time, we use the same hardware (i.e., AWS p3.16xlarge) and the same inputs (i.e., raw text, vectorized features, data split) to obtain the results of AttentionXML, X-Transformer and LightXML. The hyper-parameter of XR-Transformer and more empirical results are included in Appendix A.3]

**Model Performance.** The comparisons of Precision@k (P@k) and training time are shown in Table 2] and Table 8] respectively. The proposed XR-Transformer follows AttentionXML and LightXML to use an ensemble of 3 models, while X-Transformer uses an ensemble of 9 models [12]. More details about the ensemble setting can be found in Appendix A.3]. The proposed XR-Transformer

Table 4: Single model comparison of DNN based XMC models. Training time on p3.16xlarge with 8 Nvidia V100 GPUs  $T_{train}^8$  are reported for AttentionXML, X-Transformer and XR-Transformer, whereas time on single Nvidia V100 GPU  $T_{train}^1$  is reported for LightXML and XR-Transformer.

Dataset	Method	P@1	P@3	P@5	$T_{train}^1$	$T_{train}^8$
Wiki10-31K	AttentionXML-1	87.1	77.8	68.8	-	<b>0.5</b>
	X-Transformer-1	87.5	77.2	67.1	-	3.5
	LightXML-1	87.8	77.3	68.0	6.7	-
	<b>XR-Transformer-1</b>	<b>88.0</b>	<b>78.7</b>	<b>69.1</b>	<b>1.3</b>	<b>0.5</b>
Wiki-500K	AttentionXML-1	75.1	56.5	44.4	-	<b>12.5</b>
	X-Transformer-1	44.8	40.1	34.6	-	56.0
	LightXML-1	76.3	57.3	44.2	89.6	-
	<b>XR-Transformer-1</b>	<b>78.1</b>	<b>57.6</b>	<b>45.0</b>	<b>29.2</b>	<b>12.5</b>
Amazon-670K	AttentionXML-1	45.7	40.7	36.9	-	8.1
	X-Transformer-1	44.8	40.1	34.6	-	56.0
	LightXML-1	47.3	42.2	38.5	53.0	-
	<b>XR-Transformer-1</b>	<b>49.1</b>	<b>43.8</b>	<b>40.0</b>	<b>8.1</b>	<b>3.4</b>

framework achieves new SOTA results in **14 out of 18** evaluation columns (combination of datasets and P@k), and outperforms competitive methods on the large datasets. Next, we show the training time of XR-Transformer is significantly less than other DNN-based models.

**Training Cost.** Table 8 shows the training time for these DNN-based models. To have fair comparison, all the experiments are conducted with float32 precision on AWS p3.16xlarge instance with 8 Nvidia V100 GPUs except for LightXML, which was run on single V100 GPU since multi-GPU training is not implemented. XR-Transformer consumes significantly less training time compared with other transformer based models and the shallow BiLSTM model AttentionXML. On Amazon-3M, XR-Transformer has  $20x$  speedup over X-Transformer while achieving even better P@k. Finally, in table 4 we compare XR-Transformer with LightXML under the single model setup (no ensemble), where XR-Transformer still consistently outperforms LightXML in P@k and training time.

Table 5: Comparing XR-Transformer with Pre-Trained and word2vec embeddings concatenated with TF-IDF features.

Methods	P@1	P@3	P@5	P@1	P@3	P@5	P@1	P@3	P@5
	Eurlex-4K			Wiki10-31K			AmazonCat-13K		
TF-IDF	84.14	72.05	60.97	85.75	75.79	66.69	94.64	79.98	64.79
word2vec +TF-IDF	84.35	71.27	59.10	86.11	76.92	66.45	94.53	79.44	63.94
Pre-Trained +TF-IDF	84.92	71.40	59.36	85.78	78.30	68.33	95.05	80.12	64.53
<b>XR-Transformer</b>	<b>88.41</b>	<b>75.97</b>	<b>63.18</b>	<b>88.69</b>	<b>80.17</b>	<b>70.91</b>	<b>96.79</b>	<b>83.66</b>	<b>68.04</b>
	Wiki-500K			Amazon-670K			Amazon-3M		
TF-IDF	65.59	46.72	36.46	43.38	38.40	34.77	47.40	44.15	41.87
word2vec +TF-IDF	68.21	48.16	37.54	44.04	39.07	35.35	47.51	44.49	42.19
Pre-Trained +TF-IDF	70.18	49.82	38.75	44.55	38.91	34.77	49.66	46.41	43.96
<b>XR-Transformer</b>	<b>79.40</b>	<b>59.02</b>	<b>46.25</b>	<b>50.11</b>	<b>44.56</b>	<b>40.64</b>	<b>54.20</b>	<b>50.81</b>	<b>48.26</b>

**Comparison of Different Semantic Embeddings.** To provide more empirical justifications, that the improvement in performance comes from better semantic embedding rather than the introducing of TF-IDF features, we further tested models using Pre-Trained Transformer and word2vec embeddings concatenated with the same TF-IDF features.

Table 5 summarizes the performance of these models on all 6 datasets. In particular, word2vec is using token embedding from *word2vec-google-news-300* and for Pre-Trained we use the same setting as XR-Transformer (3-model ensemble). On large datasets such as Wiki-500K/Amazon-670K/Amazon-3M, Pre-Trained +TF-IDF has marginal improvement compared to the baseline TF-IDF features. Nevertheless, our proposed XR-Transformer still enjoy significant gain compared to Pre-Trained +TF-IDF. This suggests the major improvement is from learning more powerful neural semantic embeddings, rather than the use of TF-IDF.

**Effect of Cost-Sensitive Learning.** In Table 6, we analyze the effect of cost sensitive learning on four XMC datasets with the largest output spaces. On most datasets, cost sensitive learning via aggregated labels yields better performance than those without. We also show that cost-sensitive learning is not only beneficial to XR-Transformer, but also useful to its linear counterpart XR-Linear [7]. See Appendix A.4.1 for more results.

Table 6: Ablation of cost-sensitive learning on the single XR-Transformer model with or without Cost Sensitive (CS). Precision@1,3,5 P(@k) and Recall@1,3,5 (R@k) are reported.

Dataset	Method	P@1	P@3	P@5	R@1	R@3	R@5
Wiki10-31K	XR-Transformer-1(w/o CS)	86.8	77.6	68.8	5.2	13.6	19.8
	XR-Transformer-1	88.0	78.7	69.1	5.3	13.8	19.9
Wiki-500K	XR-Transformer-1(w/o CS)	77.6	57.4	44.9	25.8	48.1	57.8
	XR-Transformer-1	78.1	57.6	45.0	26.1	48.5	58.1
Amazon-670K	XR-Transformer-1(w/o CS)	49.1	43.8	40.0	10.3	25.6	37.7
	XR-Transformer-1	49.0	43.7	39.9	10.4	25.7	37.7
Amazon-3M	XR-Transformer-1(w/o CS)	50.2	47.6	45.4	3.4	8.4	12.4
	XR-Transformer-1	52.6	49.4	46.9	3.8	9.3	13.6

**Effect of Label Resolution and Text Representation.**

Next, we compare the effect of label resolution on the quality of the fine-tuned transformer embeddings. We fine-tune transformer models in a non-recursive manner on a two layer HLT with different leaf cluster size. Then the fine-tuned transformer embeddings are used along or in combination with TF-IDF features to produce the predictions with refined HLT. From Figure 2 we can observe that a larger cluster size will result in worse semantic features. Figure 2 also shows that combining semantic features  $\Phi_{dnn}$  with statistical features  $\Phi_{tfidf}$  could in general improve the model performance.

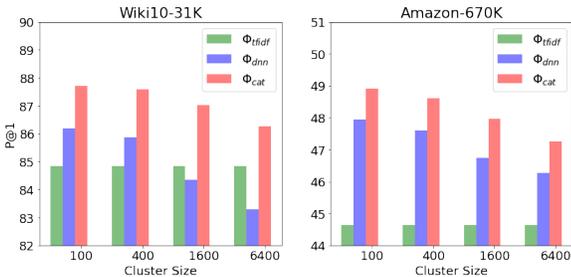


Figure 2: Comparison of BERT model fine-tuned with different label resolution. Larger cluster size means lower label resolution. Note that  $\Phi_{cat}$  is the normalized concatenation of  $\Phi_{tfidf}$  and  $\Phi_{dnn}$ .

**6 Conclusion and Future work**

In this paper, we have presented XR-Transformer approach, which is an XMC architecture that leverages multi-resolution objectives and cost sensitive learning to accelerate the fine-tuning of pre-trained transformer models. Experiments show that the proposed method establishes new state-of-the-art results on public XMC datasets while taking significantly less training time compared with earlier transformer based methods. Although the proposed architecture is designed for XMC, the ideas can be applied to other areas such as information retrieval or other DNN models such as CNNs/ResNets. Also, more extensive study is required to understand why the coarse-to-fine scheme would lead to not only faster training but better overall quality. A hypothesis is that the problem is being solved at multiple scales hence leading to more robust learning of deep transformer models.

## References

- [1] Wei-Cheng Chang, Felix X. Yu, Yin-Wen Chang, Yiming Yang, and Sanjiv Kumar. Pre-training tasks for embedding-based large-scale retrieval. In *International Conference on Learning Representations*, 2020.
- [2] Kenton Lee, Ming-Wei Chang, and Kristina Toutanova. Latent retrieval for weakly supervised open domain question answering. In *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics (ACL)*, 2019.
- [3] Yashoteja Prabhu, Anil Kag, Shrutendra Harsola, Rahul Agrawal, and Manik Varma. Parabel: Partitioned label trees for extreme classification with application to dynamic search advertising. In *WWW*, 2018.
- [4] Yashoteja Prabhu and Manik Varma. Fastxml: A fast, accurate and stable tree-classifier for extreme multi-label learning. In *KDD*, 2014.
- [5] Wei-Cheng Chang, Daniel Jiang, Hsiang-Fu Yu, Choon-Hui Teo, Jiong Zhang, Kai Zhong, Kedarnath Kolluri, Qie Hu, Nikhil Shandilya, Vyacheslav Ievgrafov, Japinder Singh, and Inderjit S Dhillon. Extreme multi-label learning for semantic matching in product search. In *KDD*. ACM, 2021.
- [6] Sujay Khandagale, Han Xiao, and Rohit Babbar. Bonsai: diverse and shallow trees for extreme multi-label classification. *Machine Learning*, 109(11):2099–2119, 2020.
- [7] Hsiang-Fu Yu, Kai Zhong, and Inderjit S Dhillon. PECOS: Prediction for enormous and correlated output spaces. *arXiv preprint arXiv:2010.05878*, 2020.
- [8] Ronghui You, Zihan Zhang, Ziyue Wang, Suyang Dai, Hiroshi Mamitsuka, and Shanfeng Zhu. AttentionXML: Label tree-based attention-aware deep model for high-performance extreme multi-label text classification. In *Advances in Neural Information Processing Systems*, pages 5812–5822, 2019.
- [9] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics (NAACL)*, 2019.
- [10] Zhilin Yang, Zihang Dai, Yiming Yang, Jaime Carbonell, Ruslan Salakhutdinov, and Quoc V Le. XLNet: Generalized autoregressive pretraining for language understanding. In *NIPS*, 2019.
- [11] Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. RoBERTa: A robustly optimized BERT pretraining approach. *arXiv preprint arXiv:1907.11692*, 2019.
- [12] Wei-Cheng Chang, Hsiang-Fu Yu, Kai Zhong, Yiming Yang, and Inderjit S Dhillon. Taming pretrained transformers for extreme multi-label text classification. In *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 3163–3171, 2020.
- [13] Ting Jiang, Deqing Wang, Leilei Sun, Huayi Yang, Zhengyang Zhao, and Fuzhen Zhuang. LightXML: Transformer with dynamic negative sampling for high-performance extreme multi-label text classification. In *AAAI*, 2021.
- [14] Wei-Sheng Lai, Jia-Bin Huang, Narendra Ahuja, and Ming-Hsuan Yang. Deep laplacian pyramid networks for fast and accurate super-resolution. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, July 2017.
- [15] Tero Karras, Timo Aila, Samuli Laine, and Jaakko Lehtinen. Progressive growing of gans for improved quality, stability, and variation. In *ICLR*, 2018.
- [16] Tero Karras, Samuli Laine, and Timo Aila. A style-based generator architecture for generative adversarial networks. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 4401–4410, 2019.

- [17] Yoshua Bengio, Jérôme Louradour, Ronan Collobert, and Jason Weston. Curriculum learning. In *Proceedings of the 26th annual international conference on machine learning*, pages 41–48, 2009.
- [18] Rohit Babbar and Bernhard Schölkopf. DiSMEC: distributed sparse machines for extreme multi-label classification. In *WSDM*, 2017.
- [19] Ian EH Yen, Xiangru Huang, Kai Zhong, Pradeep Ravikumar, and Inderjit S Dhillon. PD-Sparse: A primal and dual sparse approach to extreme multiclass and multilabel classification. In *International Conference on Machine Learning (ICML)*, 2016.
- [20] Ian EH Yen, Xiangru Huang, Wei Dai, Pradeep Ravikumar, Inderjit Dhillon, and Eric Xing. PPDsparse: A parallel primal-dual sparse method for extreme classification. In *KDD*. ACM, 2017.
- [21] Rohit Babbar and Bernhard Schölkopf. Data scarcity, robustness and extreme multi-label classification. *Machine Learning*, pages 1–23, 2019.
- [22] Anna E Choromanska and John Langford. Logarithmic time online multiclass prediction. *Advances in Neural Information Processing Systems*, 28:55–63, 2015.
- [23] Hal Daumé III, Nikos Karampatziakis, John Langford, and Paul Mineiro. Logarithmic time one-against-some. In *International Conference on Machine Learning*, pages 923–932. PMLR, 2017.
- [24] Marek Wydmuch, Kalina Jasinska, Mikhail Kuznetsov, Róbert Busa-Fekete, and Krzysztof Dembczynski. A no-regret generalization of hierarchical softmax to extreme multi-label classification. In *NIPS*, 2018.
- [25] Yashoteja Prabhu, Aditya Kusupati, Nilesh Gupta, and Manik Varma. Extreme regression for dynamic search advertising. In *Proceedings of the 13th International Conference on Web Search and Data Mining*, pages 456–464, 2020.
- [26] Kalina Jasinska-Kobus, Marek Wydmuch, Krzysztof Dembczynski, Mikhail Kuznetsov, and Robert Busa-Fekete. Probabilistic label trees for extreme multi-label classification. *arXiv preprint arXiv:2009.11218*, 2020.
- [27] Kalina Jasinska-Kobus, Marek Wydmuch, Devanathan Thiruvengkatachari, and Krzysztof Dembczynski. Online probabilistic label trees. In *International Conference on Artificial Intelligence and Statistics*, pages 1801–1809. PMLR, 2021.
- [28] Yukihiko Tagami. AnnexML: Approximate nearest neighbor search for extreme multi-label classification. In *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, pages 455–464, 2017.
- [29] Himanshu Jain, Venkatesh Balasubramanian, Bhanu Chunduri, and Manik Varma. SLICE: Scalable linear extreme classifiers trained on 100 million labels for related searches. In *Proceedings of the Twelfth ACM International Conference on Web Search and Data Mining*, pages 528–536. ACM, 2019.
- [30] Y. A. Malkov and D. A. Yashunin. Efficient and robust approximate nearest neighbor search using hierarchical navigable small world graphs. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 42(4):824–836, 2020.
- [31] Chuan Guo, Ali Mousavi, Xiang Wu, Daniel N Holtmann-Rice, Satyen Kale, Sashank Reddi, and Sanjiv Kumar. Breaking the glass ceiling for embedding-based classifiers for large output spaces. In *Advances in Neural Information Processing Systems*, pages 4944–4954, 2019.
- [32] Ruiqi Guo, Philip Sun, Erik Lindgren, Quan Geng, David Simcha, Felix Chern, and Sanjiv Kumar. Accelerating large-scale inference with anisotropic vector quantization. In *International Conference on Machine Learning*, pages 3887–3896. PMLR, 2020.
- [33] Jingzhou Liu, Wei-Cheng Chang, Yuexin Wu, and Yiming Yang. Deep learning for extreme multi-label text classification. In *Proceedings of the 40th International ACM SIGIR Conference on Research and Development in Information Retrieval*, pages 115–124. ACM, 2017.

- [34] Tharun Kumar Reddy Medini, Qixuan Huang, Yiqiu Wang, Vijai Mohan, and Anshumali Shrivastava. Extreme classification in log memory using count-min sketch: A case study of amazon search with 50m products. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.
- [35] Kunal Dahiya, Deepak Saini, Anshul Mittal, Ankush Shaw, Kushal Dave, Akshay Soni, Himanshu Jain, Sumeet Agarwal, and Manik Varma. DeepXML: A deep extreme multi-label learning framework applied to short text documents. In *Proceedings of the 14th ACM International Conference on Web Search and Data Mining*, pages 31–39, 2021.
- [36] Anshul Mittal, Kunal Dahiya, Sheshansh Agrawal, Deepak Saini, Sumeet Agarwal, Purushottam Kar, and Manik Varma. DECAF: Deep extreme classification with label features. In *Proceedings of the 14th ACM International Conference on Web Search and Data Mining*, pages 49–57, 2021.
- [37] D. Saini, A.K. Jain, K. Dave, J. Jiao, A. Singh, R. Zhang, and M. Varma. GalaXC: Graph neural networks with labelwise attention for extreme classification. In *Proceedings of The Web Conference*, April 2021.
- [38] A. Mittal, N. Sachdeva, S. Agrawal, S. Agarwal, P. Kar, and M. Varma. ECLARE: Extreme classification with label graph correlations. In *Proceedings of The ACM International World Wide Web Conference*, April 2021.
- [39] Hui Ye, Zhiyu Chen, Da-Han Wang, and Brian Davison. Pretrained generalized autoregressive model with adaptive probabilistic label clusters for extreme multi-label text classification. In *International Conference on Machine Learning*, pages 10809–10819. PMLR, 2020.
- [40] Armand Joulin, Moustapha Cissé, David Grangier, Hervé Jégou, et al. Efficient softmax approximation for gpus. In *International Conference on Machine Learning*, pages 1302–1310. PMLR, 2017.
- [41] Himanshu Jain, Yashoteja Prabhu, and Manik Varma. Extreme multi-label loss functions for recommendation, tagging, ranking & other missing label applications. In *KDD*, 2016.
- [42] Marco Pedersoli, Andrea Vedaldi, Jordi Gonzalez, and Xavier Roca. A coarse-to-fine approach for fast deformable object detection. *Pattern Recognition*, 48(5):1844–1853, 2015.
- [43] Shikun Liu, Andrew J Davison, and Edward Johns. Self-Supervised generalisation with meta auxiliary learning. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.
- [44] Charles Elkan. The foundations of cost-sensitive learning. In *International joint conference on artificial intelligence*, volume 17, pages 973–978. Lawrence Erlbaum Associates Ltd, 2001.
- [45] Chun-Liang Li and Hsuan-Tien Lin. Condensed filter tree for cost-sensitive multi-label classification. In *International Conference on Machine Learning*, pages 423–431. PMLR, 2014.
- [46] Kuan-Hao Huang and Hsuan-Tien Lin. Cost-sensitive label embedding for multi-label classification. *Machine Learning*, 106(9):1725–1746, 2017.
- [47] Hsuan-Tien Lin. Advances in cost-sensitive multiclass and multilabel classification. In *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 3187–3188, 2019.
- [48] Aditya K Menon, Ankit Singh Rawat, Sashank Reddi, and Sanjiv Kumar. Multilabel reductions: what is my loss optimising? In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.
- [49] Rong-En Fan, Kai-Wei Chang, Cho-Jui Hsieh, Xiang-Rui Wang, and Chih-Jen Lin. LIBLINEAR: a library for large linear classification. *Journal of machine learning research*, 9(Aug):1871–1874, 2008.

- [50] Sujay Khandagale, Han Xiao, and Rohit Babbar. BONSAI-diverse and shallow trees for extreme multi-label classification. *arXiv preprint arXiv:1904.08249*, 2019.
- [51] Diederik Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *Proceedings of the International Conference on Learning Representations*, 2014.

## A Appendix

### A.1 Method Overview

At a high level sketch, the XR-Transformer model consists of three components. First, text vectorizers consists of both learnable transformer based semantic vectorizer and deterministic statistical vectorizer. Second, a recursive fine-tuning curriculum with multi-resolution output signals defined by a preliminary HLT and finally, multi-layer ranking models that gives final prediction together with a refined HLT. Figure 3 gives an illustration on the training and inference pipeline of XR-Transformer.

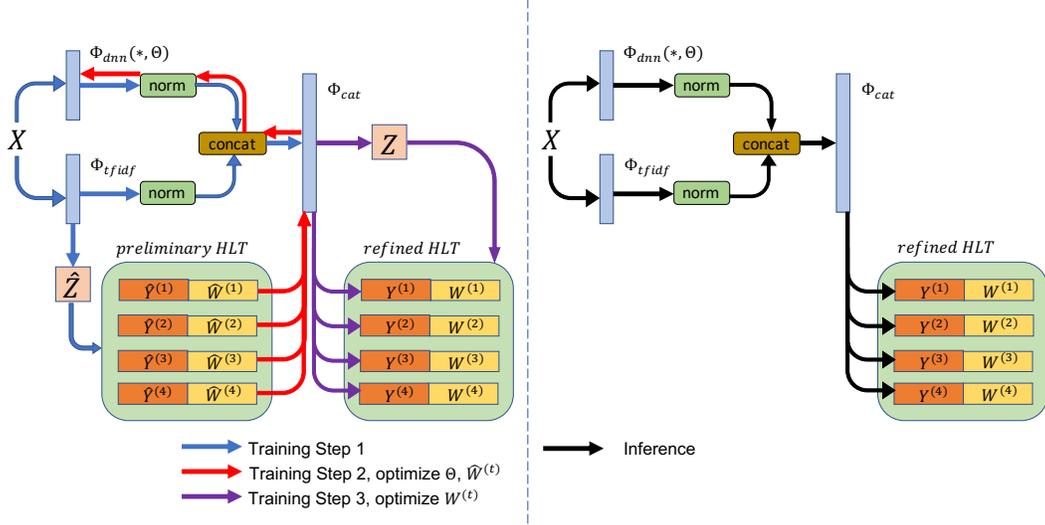


Figure 3: XR-Transformer training (left) and inference (right) architecture. XR-Transformer is trained with three steps. First, label features  $\hat{Z}$  are computed and is used to build preliminary hierarchical label tree (HLT) via hierarchical k-means. Then the transformer vectorizer  $\Phi_{dnn}(\cdot, \Theta)$  is recursively fine-tuned on multi-resolution labels  $\{\hat{Y}^{(t)}\}_{t=1}^D$ . Finally, a refined HLT is generated with  $\Phi_{cat}$  and the linear ranking models  $\{W^{(t)}\}_{t=1}^D$  are learned with refined multi-resolution labels  $\{Y^{(t)}\}_{t=1}^D$ . Only the transformer vectorizer  $\Phi_{dnn}$ , refined HLT and  $\{W^{(t)}\}_{t=1}^D$  are needed during inference.

### A.2 Evaluation Metrics

In this section, we define the evaluation metrics used in this paper. The most widely used evaluation metric for XMC is the precision at k (Prec@k) and recall at k (Recall@k), which are defined as:

$$\text{Prec@k} = \frac{1}{k} \sum_{l=1}^k y_{rank(l)} \quad (12)$$

$$\text{Recall@k} = \frac{1}{\sum_{i=1}^L y_i} \sum_{l=1}^k y_{rank(l)} \quad (13)$$

where  $y \in \{0, 1\}^L$  is the ground truth label and  $rank(l)$  is the index of the  $l$ -th highest predicted label.

For performance comparison on tail labels, we also report propensity scored precision (PSP@k), which is defined as:

$$\text{PSP@k} = \frac{1}{k} \sum_{l=1}^k \frac{y_{rank(l)}}{p_{rank(l)}} \quad (14)$$

where  $p_{rank(l)}$  is the propensity score at position  $rank(l)$  [41]. The metric involves application specific parameters  $A$  and  $B$ . For consistency, we use the same setting as AttentionXML [8] for all datasets.

### A.3 Model Hyperparameters

For each sub-XMC problem, XR-Transformer fine-tunes the transformer encoder with Adam [51] with linear learning rate schedule and a batch size of 32 per GPU (256 total). The dropout probability is set to be 0.1 for all models and bootstrapping [11] is used for all fine-tuning problems except for the root layer. The detailed hyperparameters are listed in Table 7

#### A.3.1 Model Ensemble Setup

For AttentionXML, LightXML and X-Transformer, we use the same ensemble setting provided in the paper. In particular, AttentionXML uses ensemble of 3 models, LightXML uses ensemble of 3 transformer encoders and X-Transformer uses 9 model ensemble with BERT, RoBerta, XLNet large models with three difference indexers. For our method, we follow the setting of LightXML and use the ensemble of BERT, RoBerta and XLNet for Eurlex-4K, Wiki10-31K and AmazonCat-13K, and ensemble of three BERT model for Wiki-500K, Amazon-670K and Amazon-3M.

Table 7: Hyperparameters for XR-Transformer.  $HLLT_{prelim}$  and  $HLLT_{refine}$  define the structures of the preliminary and refined hierarchical label trees.  $lr_{max}$  is the maximum learning rate used in fine-tuning.  $n_{step}$  is the total number of optimization steps across the multi-resolution fine-tuning.  $N_x$  is the number of input tokens after text truncation.  $\alpha$  is the hyper-parameter for cost sensitive learning.  $\lambda$  is the weight for the regularization term.

Dataset	$HLLT_{prelim}$	$HLLT_{refine}$	$lr_{max}$	$n_{step}$	$N_x$	$\alpha$	$\lambda$
Eurlex-4K	16-256-3956	4-32-256-3956	$5 \times 10^{-5}$	2400	128	1.0	0.5
Wiki10-31K	128-2048-30938	8-128-2048-30938	$1 \times 10^{-4}$	4000	256	0.25	0.25
AmazonCat-13K	128-1024-13330	128-1024-13330	$1 \times 10^{-4}$	45000	256	2.0	2.0
Wiki-500K	64-512-4096-32768	8-256-8192-501070	$1 \times 10^{-4}$	60000	128	0.25	0.25
Amazon-670K	128-2048-32768	8-256-8192-670091	$1 \times 10^{-4}$	20000	128	-	1.0
Amazon-3M	128-2048-32768	8-256-8192-2812281	$1 \times 10^{-4}$	30000	128	0.125	0.125

### A.4 More Empirical Results

Table 8: Comparing training time (in hours) of DNN-based methods that produce the SOTA results in Table 2. The number following the model indicates the number of ensemble models used.

Dataset	AttentionXML-3	X-Transformer-9	LightXML-3	XR-Transformer-3
Eurlex-4K	0.9	7.5	16.9	<b>0.8</b>
Wiki10-31K	<b>1.5</b>	14.1	26.9	<b>1.5</b>
AmazonCat-13K	24.3	147.6	310.6	<b>13.2</b>
Wiki-500K	<b>37.6</b>	557.1	271.3	38.0
Amazon-670K	24.2	514.8	159.0	<b>10.5</b>
Amazon-3M	54.8	542.0	-	<b>29.3</b>

#### A.4.1 Cost-sensitive Learning

In table 9, we show that the cost-sensitive learning via recursive label aggregation is beneficial to both the linear XR-Linear and the Transformer-based XR-Transformer model. On most datasets, cost sensitive learning yields better performance.

#### A.4.2 Inference Speed

We report the inference time for AttentionXML, X-Transformer, LightXML and XR-Transformer on XMC datasets in table 10. The inference results (millisecond per sample) are evaluated on single GPU and single CPU for most comparing models except for AttentionXML, which is evaluated with multi-GPUs on Wiki-500K, Amazon-670K and Amazon-3M. AttentionXML requires model-parallelism on those largest datasets otherwise it may be out-of-memory on a single-GPU setup.

Table 9: Ablation of cost-sensitive learning on the single XR-Linear and XR-Transformer model with or without Cost Sensitive (CS). Precision@1,3,5 (P@k) and Recall@1,3,5 (R@k) are reported.

Dataset	Method	P@1	P@3	P@5	R@1	R@3	R@5
Wiki10-31K	XR-Linear-1(w/o CS)	84.5	73.1	64.1	5.0	12.8	18.4
	XR-Linear-1	85.7	75.0	65.2	5.1	13.1	18.7
	XR-Transformer-1(w/o CS)	86.8	77.6	68.8	5.2	13.6	19.8
	XR-Transformer-1	88.0	78.7	69.1	5.3	13.8	19.9
Wiki-500K	XR-Linear-1(w/o CS)	66.7	47.8	37.3	21.7	39.5	47.6
	XR-Linear-1	67.7	48.4	37.6	22.2	40.4	48.6
	XR-Transformer-1(w/o CS)	77.6	57.4	44.9	25.8	48.1	57.8
	XR-Transformer-1	78.1	57.6	45.0	26.1	48.5	58.1
Amazon-670K	XR-Linear-1(w/o CS)	44.0	39.2	35.4	9.2	22.7	33.2
	XR-Linear-1	44.4	39.3	35.6	9.4	23.0	33.6
	XR-Transformer-1(w/o CS)	49.1	43.8	40.0	10.3	25.6	37.7
	XR-Transformer-1	49.0	43.7	39.9	10.4	25.7	37.7
Amazon-3M	XR-Linear-1(w/o CS)	46.8	44.0	41.9	2.9	7.3	10.7
	XR-Linear-1	50.1	46.6	44.0	3.4	8.4	12.2
	XR-Transformer-1(w/o CS)	50.2	47.6	45.4	3.4	8.4	12.4
	XR-Transformer-1	52.6	49.4	46.9	3.8	9.3	13.6

Table 10: Comparison of XR-Transformer with recent XMC methods on public datasets w.r.t. inference time. Times are recorded with single Nvidia V100 GPU and batch size of 1 except for the numbers with superscript \*, where model parallel was used and inference was done with 8 GPUs. The unit is milliseconds per sample.

Dataset	AttentionXML-1	X-Transformer-1	LightXML-1	XR-Transformer-1
Eurlex-4K	12.7	48.2	24.7	22.3
Wiki10-31K	20.0	48.1	27.1	39.1
AmazonCat-13K	14.4	47.6	24.1	26.1
Wiki-500K	80.1*	48.1	27.3	33.9
Amazon-670K	76.0*	48.0	23.3	30.9
Amazon-3M	130.5*	50.2	-	35.2

### A.4.3 Propensity-score Precision

We report the propensity scored precision (PSP@k) metric on large scale XMC datasets for PfastreXML, Parabel, AttentionXML and XR-Transformer in Table 11. For consistency, we use the same setting as AttentionXML [8] for all datasets.

Table 11: Comparison of XR-Transformer with recent XMC methods on 3 large public datasets w.r.t. PSP@k (propensity scored precision at  $k = 1, 3, 5$ ). Results with a trailing reference are taken from [8] Table 6]. We obtain the results of AttentionXML\* and XR-Transformer on the same vectorized feature matrix provided in [8] and same hyper-parameter for propensity score calculation.

Methods	Wiki-500K			Amazon-670K			Amazon-3M		
	PSP@1	PSP@3	PSP@5	PSP@1	PSP@3	PSP@5	PSP@1	PSP@3	PSP@5
PfastreXML [41]	32.02	29.75	30.19	20.30	30.80	32.43	<b>21.38</b>	23.22	24.52
Parabel [3]	26.88	31.96	35.26	26.36	29.95	33.17	12.80	15.50	17.55
AttentionXML*	30.69	38.92	44.00	30.25	33.88	37.18	15.42	18.32	20.48
XR-Transformer*	<b>35.76</b>	<b>42.22</b>	<b>46.36</b>	<b>36.16</b>	<b>38.39</b>	<b>40.99</b>	20.52	<b>23.64</b>	<b>25.79</b>

## A.5 Potential Negative Societal Impacts

This paper focus on the acceleration of the training algorithms on XMC. To the best of our knowledge, our work poses no negative societal impacts.

## Checklist

1. For all authors...
  - (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
  - (b) Did you describe the limitations of your work? [Yes] See Section 6
  - (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section A.5
  - (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
  - (a) Did you state the full set of assumptions of all theoretical results? [N/A]
  - (b) Did you include complete proofs of all theoretical results? [N/A]
3. If you ran experiments...
  - (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
  - (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section A.3
  - (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [No]
  - (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Section 5
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
  - (a) If your work uses existing assets, did you cite the creators? [Yes]
  - (b) Did you mention the license of the assets? [No]
  - (c) Did you include any new assets either in the supplemental material or as a URL? [Yes]
  - (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [No]
  - (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [No]
5. If you used crowdsourcing or conducted research with human subjects...
  - (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
  - (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
  - (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]