IRLI: Iterative Re-partitioning for Learning to Index

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Abstract
Neural models have transformed the fundamental information retrieval problem of mapping a query to a giant set of items. However, the need for efficient and low latency inference forces the community to reconsider efficient approximate near-neighbor search in the item space. To this end, learning to index is gaining much interest in recent times. Methods have to trade between obtaining high accuracy while maintaining load balance and scalability in distributed settings. We propose a novel approach called IRLI (pronounced ‘early’), which iteratively partitions the items by learning the relevant buckets directly from the query-item relevance data. Furthermore, IRLI employs a superior power-of-k-choices based load balancing strategy. We mathematically show that IRLI retrieves the correct item with high probability under very natural assumptions and provides superior load balancing. IRLI surpasses the best baseline’s precision on multi-label classification while being 5x faster on inference. For near-neighbor search tasks, the same method outperforms the state-of-the-art Learned Hashing approach NeuralLSH by requiring only ≈ 1/6 of the candidates for the same recall. IRLI is both data and model parallel, making it ideal for distributed GPU implementation. We demonstrate this advantage by indexing 100 million dense vectors and surpassing the popular FAISS library by > 10% on recall.

1. Introduction
For a given query q, the classical problem in information retrieval (IR) is to learn a function f that maps q to one (or few) of an extensive set (often hundreds of millions) of discrete item sets. Most practical applications in IR have data with only the query-item relevance (like the classical query-product purchase data (Nigam et al., 2019; Medini et al., 2019)). Modern search engines often deploy a pipeline in which queries and items are first embedded into a dense vector space. Here the information retrieval problem gets reduced to the Approximate Near Neighbor (ANN) search in the embedding space. Analogs of this approach are explored in industry-scale works like SLICE (Jain et al., 2019) (Bing Search) and DSSM (Nigam et al., 2019) (Amazon Search). Approximate Near Neighbor (ANN), being one of the most studied algorithms in machine learning, is still far from being solved to a satisfactory extent in the context of information retrieval. In the past decade, learning-based solution for ANN has shown significant promise. Surprisingly, learning-based ANN is precisely the same information retrieval problem of finding the function f that maps q to one (or few) of an extensive set (often hundreds of millions) of discrete neighbors. The hardness of the fact that we are dealing with a large item set remains the primary challenge.

Learning to index has been a sought-after solution to the fundamental challenge of large item space, particularly in the context of Approximate Near Neighbor (ANN) search (Kraska et al., 2018). The idea behind learning to index is to find a function f that maps the query q to a reasonably sized B discrete partitions, where B is much smaller than the number of total items L. The hope is that if the partitions are reasonably balanced, then the function f reduces the search space from L to L/B, which is manageable for large enough B.

Several approximate algorithms have been proposed for learning to index. These algorithms reduce the search space, mainly using space partitioning (Dong et al., 2019) or graph-based methods (Malkov and Yashunin, 2018), or by reducing the complexity of distance computation such as quantization and lookup table based methods (Johnson et al., 2019). Graph-based NNS methods are efficient but limited to small-scale datasets. Due to their sequential nature, it is not trivial to parallelize the query and indexing process. Given this, many commercial applications that deal with large-scale data increasingly use partitioning based approaches.

Overall, the current IR pipeline still struggles with two significant challenges - 1) Learning embedding from query-item relevance is a pairwise training process leading to a
massive amount of training samples and extended training time. Additionally, negative sampling techniques have to be employed to prevent degenerate solutions, which would only exacerbate the problem for large output spaces. 2) The power-law distribution of data causes an imbalanced portion of items into the hash buckets. As a result, frequently queried items tend to coalesce in large numbers into a few buckets, leaving the infrequent ones in the remaining buckets. This imbalance leads to higher inference times as we query heavy buckets more often than the lighter ones.

1.1. Our contributions

1) We propose a learning-to-index algorithm - IRLI, which learns to partition and map together using a single neural network via an alternative training and re-partitioning.

2) We theoretically show that IRLI achieves superior recall while maintaining load-balance in convergence.

3) We surpass the best Learned Indexing baselines on recall by probing < 20% candidates. We outperform the best Extreme Classification baselines on precision while inferring 5× faster.

4) We index a 100MM sample of the Deep-1B dataset by a trivial distribution of the vectors across eight nodes. With a 4 ms latency on CPU, we achieve a recall of 90%, which is a good 10% over the popular FAISS library.

2. Related works

There are several well-known approaches for partitioning like k-means clustering (Wang and Su, 2011), locality sensitive hashing (LSH) (Shrivastava and Li, 2014; Andoni et al., 2015; Lv et al., 2007) and tree-based methods like PCA trees (Sproul, 1991) and Randomised Partition trees (Dasgupta and Sinha, 2013). LSH in particular is a cheap and fast solution for high-dimensional data indexing. However, both LSH and k-means generate partitions that have extremely skewed load for lop-sided distributed data. The tree-based methods on the other hand suffer from the curse of dimensionality. Additionally, their hierarchical design diminishes their parallelism during the query and construction process.

The power law distribution issue in traditional indexing has warranted research in load-balanced indexing schemes. An early attempt in this regard is Balanced K-Means (Malinen and Fränti, 2014), which has high construction time dampening its scalability. A recent noteworthy work is NeurallSH (NLSH) (Dong et al., 2019), which uses KaHIP (Sanders and Schulz, 2013), a balanced graph-partitioning algorithm. NLSH maps a query to the relevant partition/partitions via a brute force approach, using the partition-centers’ distance with the query. However, the centroids do not always reflect the higher-order statistics of the partitions. Sometimes, they do get drifted by outliers within the partitions. NLSH learns a model to rank the partitions generated by the k-NN graph. Learning improves the mapping by training on the true query to partition affinity.

Parabel: In the context of Information Retrieval, Parabel (Prabhu et al., 2018) is one of the primary algorithms that partitions the label space into roughly equal sets via a balanced 2-means label tree, where the label vectors are constructed using input instances. Subsequent improvements like eXtremeText (Wydmuch et al., 2018) and Bon sai (Khandagale et al., 2020) relax the 2-way partitioning to higher orders of hierarchy.

SLICE: Another recent work, SLICE, builds an ANN graph on the label vectors obtained from a pre-trained network. It maps a query to the common embedding space during inference and performs a random walk on the ANN graph to obtain the relevant labels.

All existing approaches decouple the partitioning step from the learning step. Once a partition is created, it is fixed for the rest of the process while we map the query using either centroids, hashing, or a learned model. In many cases, the partitioning process is an off-the-shelf algorithm (like KaHIP). Our work differs from the prior work primarily in the fact that we alternatively learn both the mapping and partitions. We have a single model that maps the query to buckets and also partitions the labels for subsequent training. To improve the candidate set precision, we repeat this process in few independent repetitions.

3. Our Method: IRLI

Iterative Re-partitioning for Learning to Index (IRLI) begins with a random-pooling based index initialization followed by an iterative process of alternating train and re-partition steps. We train R independent such indexes and use them for efficient item retrieval. Figures 1 and 2 illustrate our algorithm with a toy example of 5 buckets.

Notation: For a given dataset D, we denote a query vector by x and its labels by y. Let N be the total number of train vectors, d be the input vector dimension, and L be the total number of labels. For the ANN scenario, \( L = N \). \( R \) is the number of repetitions (independent indexes), \( B \) is the number of partitions in each repetition, and \( f(.) \) is the learned deep-net model (we have \( R \) such models).

3.1. Initialization:

We initialise the partitioning randomly. For this, we use \( R \) 2-universal hash functions \( h_r : [L] \rightarrow [B] \), \( r \in \{1, 2, ..., R\} \). The hash function \( h_r(.) \) uniformly maps the \( L \) labels into \( B \) buckets. As the pooling is randomised, the buckets contain an equal number of labels in expectation. If the application is near neighbor, the \( N \) vectors gets pooled randomly \( R \).
We have while a smaller $K$ ensures higher precision and recall.

### 3.2. Alternative Training and Re-partitioning:

**Training:** We train a feed forward neural network to learn the affinity $f_l$ of a given point $x$ to $B$ buckets where $B < L$. We have $R$ independent partitions and thereby $R$ independent neural networks \{$(f_r, \forall r \in \{1, 2, \ldots, R\})$\}. We are effectively solving a classification problem using the binary cross-entropy loss

$$\mathcal{L}(x, y, B) = - \sum_{b=1}^{B} y_{o,b} \log(p_b) - (1 - y_{o,b}) \log(1 - p_b)$$

by providing $B$ softmax scores ($p_b$) against the ground-truth one hot value ($y_{o,b}$). $y_{o,b} = 1$ if there is at-least one true label present in the bucket $b$, else $y_{o,b} = 0$.

In Extreme Multi-Label (XML scenario), the true labels are provided with the data. For the ANN datasets, we use the 100 exact near neighbors to a query point (using the corresponding distance metric) as labels. These neighbors have to be generated beforehand.

**Re-partitioning:** This is the critical step in IRLI as it creates a partition with more relevant label affinity than the current partition. Let us first define label affinity for both the XML and ANN scenarios. The label affinity in the absence of a label vector (XML scenario) is defined as:

**Definition 1** For a given label $l$ and a network $f(\cdot)$ with $B$ outputs, trained on a dataset $x, y \in \mathcal{D}$, the label affinity is given by

$$P_l = \sum_{\forall i \in y_l} f(x_i), f(.) \in R^B$$

When the label vector is given (ANN scenario) the label affinity is defined as:

**Definition 2** For a given label embedding $\mathbf{l}$ and a network $f(.)$ with $B$ outputs, the label affinity is given by

$$P_l = f(\mathbf{l}), f(.) \in R^B$$

Please refer to section 4 for further analysis on the label affinity behavior.

Once the training is done, a label ($l \in \{1, 2, \ldots, L\}$) is re-partitioned by assigning it to its top affinity bucket ($\text{argmax} P_l$), in each of the $R$ repetitions. It is important to note that, for similar labels, the network will provide very similar label affinities.

**Load Balancing:** In general, a real dataset does not have a uniform distribution. Consequently, similarity-based partitioning leads to an unbalanced load across the buckets. To
overcome this, we select *K* top affinity buckets for each label instead of 1. We choose the least occupied bucket among these top-scoring buckets and assign the label to it. This ensures that the label fills the lighter bucket first to keep up with the load of the top buckets of similar labels. As we observe later in section 5, we will only need a small *K* to maintain a near-perfect load balance. For example, on GloVe100 dataset, for *B* = 5000, we only need *k* = 10 buckets to achieve a load variance of approx 3 as compared to 15 for random bucket assignment (lower the load-variance, better the balance).

**Absence of label embedding:** In the case of ANN datasets, label vectors are given beforehand. On the other hand, if a label embedding is not given, we need an equivalent of it to pass through the learned network and get the label affinity. For such cases, we retrieve the bucket scores for a label using its data points (as shown in definition 1). For each label *l*, we use the sum of the corresponding data vectors’ softmax probability.

We re-assign labels once every few training epochs (once every five epochs in our experiments). We alternate between the training and re-partitioning steps until the number of new assignments converges to zero.

**3.3. Inference/Query:**

After training, we store the trained models and inverted indexes for all *R* repetitions. During the query process, a vector *q* ∈ *R*^d^ is passed through *R* trained nets independently in parallel, where each one gives a *B* dimensional probability vector.

We select the top-*m* buckets (*m* = 5 – 10 if *B* is around 5000) from each model. This gives a total of *m* × *R* buckets to probe. A union of points/labels in these buckets is the target candidate set. Additionally, we count each candidate’s frequency of occurrence in the total *m* × *R* sets. A higher frequency of a candidate label signifies a higher relevance to the query point. In the end, we keep only the higher relevance candidates by filtering and rejecting the candidates below a certain frequency threshold from the pool. Please refer to Figure 2 for an illustrative view of the query process.

**Two crucial points to note:** 1) Our procedure will ensure that every network has δ higher probability of selecting a relevant label than it can with learning on any predefined random partitioning. We prove this in section 4. 2) Candidate set selection from *R* repetition and frequency-based filtering exponentially decrease the variance of our true labels estimates. This is analyzed further in Appendix.
4. Analysis

In this section, we theoretically analyze IRLI from two main perspectives. First, we show that the predicted probability of buckets corresponding to the relevant labels increases after re-assigning the labels. Second, analogous to the popular power-of-2-choices, we show that the process of re-assigning to the least occupied of the top-$K$ buckets is the optimal strategy to ensure load balance across the buckets.

As mentioned before, we have $L$ classes being hashed to $B$ buckets using a universal hash function. This randomly partitions the classes into $B$ meta-classes. We estimate the top bucket probability $\max Pr(b/x)$ for a input vector $x$, where $b \in \{1,2,..B\}$. Since each of the $R$ repetitions is an instantiation of the same process, we only need an $R$-agnostic proof for the fact that re-assignment enhances the prediction probability of the most relevant bucket.

**Theorem 1** For a given dataset with $x \in \mathbb{R}^{N \times d}$, and its label $l$, the expected affinity of the input query point $x$ with $l$ increases by a margin of $\delta > 0$ after re-partitioning, i.e.,

$$E(P'_{x,h'(l)}) = E(P_{x,h(l)}) + \delta$$

where $P_x \in \mathbb{R}^B$ is the bucket affinity vector of $x$.

The increment in the query affinity, results in increment of quality of the retrieved labels.

**Proof** Let $x$ be an input vector whose label set is $\bar{y}$. Let $p_l$ denote the probability of $l$ being a true label to $x$.

Let the current partitioning be given by a mapping $h(l)$, where $h(l) \in \{1,2,...,B\}$. Also, assume $l_1, l_2 \in \bar{y}$ and $l_3 \notin \bar{y}$.

The affinity score of $x$ for $h(l_1)^{th}$ bucket is given by the summation of probability of label $l_1$ and probability of other labels in the same bucket, i.e.,

$$P_{x,h(l_1)} = p_{l_1} + \sum_{k \neq l_1} 1_{h(k) = h(l_1)}p_k$$

1 is the indicator function. Now, let us reassign the labels as per section 3.2. Let the new partition be given by $h'(l)$. If $h(l_1) \neq h(l_2)$ and $h(l_1) = h(l_3)$, we want the re-partitioning to reverse this adversarial scenario, i.e., we expect that

$$h'(l_1) = h'(l_2) \text{ and } h'(l_1) \neq h'(l_3)$$

Let $Z$ represent the event of $l_3$ being removed from $l_1$’s bucket and $l_2$ being added to it.

$$P'_{x,h'(l_1)} = p_{l_1} + \sum_{k \neq l_1} 1_{h'(k) = h'(l_1)}p_k + 1_Z(p_{l_2} - p_{l_3})$$

Expected affinity is given by-

$$E(P_{x,h'(l_1)}) = E(P_{x,h(l_1)}) + E(Z)(p_{l_2} - p_{l_3})$$

As $l_1$ and $l_2$ are high scoring label of data point $x$, $p_{l_1} = p_{l_2} > p_{l_3}$. Also $E(Z) > 0$ when there is a possible reassignment. and hence

$$E(P_{x,h'(l_1)}) = E(P_{x,h(l_1)}) + \delta$$

where $\delta > 0$.

The main implication of the above theorem is that the bucket containing the relevant label $p_{l_1}$ gets higher aggregated affinity as it will have other true labels with higher probability. It is important to note that this affinity increment is only manifested after retraining on this new partitioning of the labels. The re-partitioning alone does not affect any affinity learned by the neural net.

The increased affinity directly increases the recall during the evaluation. Given $R$ reps, the estimated affinity of $x$ is given by $P_x = \frac{1}{R} \sum_{r=1}^{R} P_r x$. With increasing $R$ the error in correct label estimation also decreases exponentially.

The same holds for the ANN scenario where the labels are the near true neighbors generated for the IRLI indexing.

**Theorem 2** Consider the process where at each step, a label is chosen independently and uniformly at random and is inserted into the index. Each new label $l$ inserted in the index chooses $K > K_0$ possible destination bins which are the top-$K$ indices of $P_l$, and is placed in the least full of these bins. For a sufficiently large $t$, the most crowded bin at time $t$ contains fewer than $\frac{\log(\log(L) + f_1(K))}{\log(K)} + O(1) + f_2(K)$ labels with high probability, where $f_1$ and $f_2$ are monotonically decreasing functions of $K$.

**Proof**: Proof of this theorem is given in Appendix. It draws parallels from the popular power-of-2-choices framework (Mitzenmacher, 2001).

5. Experiments

5.1. Multi-label Classification

**Datasets**: We use the dense versions of Wiki-500K and Amazon-670K (Jain et al., 2019) datasets available on the Extreme classification repository (Bhatia et al., 2016). The sparse versions of these datasets were scaled down and densified using XML-CNN (Liu et al., 2017) features. Both the datasets have 512 dimension vectors. Wiki-500K has 501,070 classes with 1,646,302 train points and Amazon-670K has 670,091 classes with 490,449 train points.
IRLI

| Method                              | Wiki-500K | Amazon-670K |
|-------------------------------------|-----------|-------------|
|                                     | P@1      | P@3        | P@5      | P@1      | P@3        | P@5     |
| Neural Indexing (10 buckets)        | 60.77    | 46.09      | 43.49    | 35.56    | 32.68      | 31.02   |
| Neural Indexing (5 buckets)         | 60.69    | 45.78      | 43.15    | 35.13    | 32.20      | 30.58   |
| SLICE                               | 59.89    | 39.89      | 30.12    | 37.77    | 33.76      | 30.7    |
| Parabel                             | 59.34    | 39.05      | 29.35    | 33.93    | 30.38      | 27.49   |
| AnnexML                             | 56.81    | 36.78      | 27.45    | 26.36    | 22.94      | 20.59   |
| Pfastre XML                         | 55.00    | 36.14      | 27.38    | 28.51    | 26.06      | 24.17   |
| SLEEC                               | 30.86    | 20.77      | 15.23    | 18.77    | 16.5       | 14.97   |

Table 1. Precision @1, @3, @5 for N-Index on Wiki-500K and Amazon-670K vs popular Extreme Classification benchmarks.

| Dataset     | Wiki-500K | Amazon-670K |
|-------------|-----------|-------------|
| N-Index (m=10) | 0.56     | 1.08        |
| N-Index (m=5)  | 0.47     | 0.76        |
| SLICE        | 1.37     | 3.49        |
| Parabel      | 2.94     | 2.85        |
| PfastreXML   | 6.36     | 19.35       |

Table 2. Inference speeds against the fastest Extreme Classification benchmarks.

**Network Parameters:** Each of the $R = 32$ models has an input layer of 512 dimensions, a hidden layer of 1024 dimensions, and an output layer of $B = 20000$. We train these networks for 30 epochs and re-assign the labels every five epochs.

**Metrics:** We measure precision at 1,3,5 (denoted by P@1, P@3,P@5). As there are no label vectors provided, we use the corresponding points for each label to re-partition (as explained in section 3). Here we pay an additional re-partitioning cost of $O(L)$.

**Hardware and framework:** The experiments were done on a DGX machine with 8 NVIDIA-V100 GPUs. We train with TensorFlow (TF) v1.14 library. We use TF Records data streaming to reduce GPU idle time.

**Baselines:** We compare IRLI with Parabel (Prabhu et al., 2018), SLICE (Jain et al., 2019), AnnexML (Tagami, 2017), Pfast XML (Jain et al., 2016) and SLEEC (Bhatia et al., 2015).

**Results:** Tables 1 and 2 provide the precision and inference time comparison of 2 IRLI variants ($m = 5$ and $m = 10$) with all the baselines. We analyze the precision and runtime during inference after selecting the top $m = 5$, 10 buckets from each of the 32 independent indexes. While the best labels are expected to be present in the topmost bucket, we relax this by querying the top 5/10 buckets per index. We can observe that IRLI Index gives the best precision and runtime, beating all baselines for Wiki-500k dataset. On the Amazon-670K, it is faster and more precise on P@5 metric than the baselines in comparison.

**5.2. Nearest Neighborhood Search**

**Dataset:** We have used two million-scale datasets from ANN benchmarks (Aumüller et al., 2020)- Glove100 (Pennington et al., 2014) and Sift1M. Glove100 has total 1,183,514 points, each a 100 dimensional vector and trained with angular distance metric. Sift-1M has exactly 1 MM points, each a 128 dimensional vector and trained with the euclidean distance metric.

**Hyper-parameters:** Each of the $R$ models are simple feed forward networks with an input layer of 100 or 128 (Glove vs SIFT), one hidden layer of 1024 neurons and and output layer of $B = 5000$.

**Hardware and framework:** The experiments were done on a DGX machine with 8 NVIDIA-V100 GPUs. We train with Tensorflow (TF) v1.14 library. We use TF Records data streaming to reduce GPU idle time.

**Baselines:** We compare IRLI against the popular learned partitioning methods like Neural LSH, kmeans+Neural Catalyzer (Sablayrolles et al., 2018) and Cross-Polytype LSH. All baselines are measured with and without hierarchy (1-level and 2-level). Please refer to figure 3 for the detailed comparison plots. For every baseline in the figure, a tag of $1-256$ denotes 1 level, 256 buckets, while a tag of $2-256$ denotes two levels, 256 buckets (65536 leaf nodes effectively).

**Metrics:** Our metric of interest is the recall of the top 10 neighbors for a particular candidate size. To be precise,
IRLI

5.2.1. Ablation Study

**Load-Balance:** As mentioned earlier, $K = 10$ is an empirical sweet spot for retaining precision while ensuring load-balance during bucket re-assignment. Table 3 shows the standard deviation of the bucket load for Glove100 for various values of $K$. We start with a random partition of points (using a 2-universal hash function) and train for 5 epochs, after which we reassign the 1.2 M vectors as explained before. We can observe that as $K$ increases, each bucket has nearly the same number of candidates. However, a larger $K$ might compromise the relevance of buckets. Hence we chose $K = 10$ as an appropriate trade-off.

| Random Partition | K=5 | K=10 | K=25 |
|------------------|-----|------|------|
| 15.3             | 17.08 | 2.66 | 0.46 |

Table 3. Standard Deviation of load vs $K$ for Glove-100 with $B = 5000$ (mean = 236.7). Larger $K$ gets better load balance while smaller $K$ gets better precision and recall. Although $K = 25$ achieves near perfect load balance, $K = 10$ is the practical choice for all our experiments for better precision.

**Epoch-wise Performance:** Figure 4 shows the epoch-wise recall for Glove100 dataset. We can observe that the recall converges after epoch 25, justifying our choice to train for 30 epochs. The improvement in recall as we increase $R$ from 16 to 32 is significant. Beyond $R = 32$, we do not observe any considerable gain with more repetitions.

Further, keeping $R = 32$ and probing top $m = 100$ buckets for a point in each repetition, we measure the number of candidates that appear in at least 4 of the 32 repetitions. As we train more, we expect this candidate set to increase in size as we group more relevant candidates together. Table 4 confirms that trend.

5.3. Data and Model Distributed KNN on 100M points

This section demonstrates the scalability of IRLI by partitioning a 100MM subsample of Deep-1B dataset (Babenko...}

Figure 3. Above: Comparison of IRLI with other partitioning methods on Glove100 dataset: The red curve represents Recall10@10 vs the number of candidates (number of true distance computations) for IRLI. The blue lines represent different variants of the primary baseline NLSH. The best variant of NLSH (2 level-256 bins, 65536 leaf nodes) has no reported recall at larger candidate sizes. All baselines have results at both 1-level and 2-level hierarchies. Balanced k-means, LSH and Catalyst, are noticeably worse than IRLI and NLSH. Below: Comparison of IRLI with other partitioning methods on SIFT128 dataset. All baselines, including the SOTA NLSH have noticeably worse recall than IRLI.

**Results** Figure 3 show the comparison with Neural-LSH and other baselines. We can notice that the IRLI (red curve) comfortably surpasses all baselines for a given candidate size. The only baseline configuration that comes close to IRLI is NLSH with a 2-level 256 bin configuration, where the 2nd level has 65536 classes and uses k-means clustering instead of a neural network prediction.
Table 4. Candidates appearing at least 4 of 32 repetitions.

and Lempitsky, 2016) and achieving $\text{sub} - 5 \ms$ latency with a $R10@10$ of 96.16%. In the prior cases, each of the $R$ independent models catered to the entire set of labels/data points. In this case, we distribute the 100MM points across $P = 8$ disjoint nodes. This choice of $P$ nodes was made to maximize the use of all GPUs on our machine.

Dataset: Deep-1B is an image indexing dataset comprising of 1 billion 96-dimensional image descriptors. These descriptors were generated from the last layer of a pre-trained convolutional neural network as discussed in (Babenko and Lempitsky, 2016). Indexing datasets of this scale is an uphill task and the primary GPU friendly algorithm that accomplishes this is the popular FAISS library (Johnson et al., 2019).

Deep-1B also provides 350 MM additional training vectors of which we subsample 10 MM vectors to train all models across the 8 nodes.

Hyper-parameters and distribution details: As mentioned earlier, each of the 8 nodes caters to only 12.5 MM points. For each node, these 12.5 MM points are partitioned into $B = 20000$ buckets. Unlike the previous cases ($R = 32$), we choose $R = 4$ for each node. This would again lead to a total of $P \times R = 32$ models. Each model is a simple feed-forward network with an input dimension of 96 and a hidden layer with 1024 neurons. We train for a total of 20 epochs and reassign the points to the buckets once every 5 epochs.

Hardware and framework: We use a server equipped with 64 CPU cores and 8 Quadro GPUs each with 48 GB memory. However, our 32 models have a combined parameter set of 660MM float32 values requiring just 2.56 GB of GPU memory (and 2x auxiliary momentum parameters for Adam optimizer). Like with the previous cases, we train using Tensorflow v1.14.

Results: Figures 5 and 6 compare IRLI against FAISS (Johnson et al., 2019) on GPU and CPU respectively (please note the IRLI uses GPU only for the neural network prediction. Rest of the aggregation process is done entirely on CPU). We can observe that FAISS plateaus at 0.8 recall (corroborated by the reported result in (Johnson et al., 2019) too). FAISS does product quantization on the 96 dimensions data vectors using 65536 clusters. In Figure 5, $PQ32$ refers to a 32 splits of a data vector while $PQ48$ refers to a 48 split. Each vector of the codebook is a byte long. Higher-order splits yield poor recall while $PQ96$ (a quantized version of full product computation) ran out of memory on our GPU. During inference, the recall vs. time trade-off is governed by $m$ (the number of top-scoring buckets that we probe among the $B$). The red curve in figure 5 goes from an inference time of 0.637 ms to 4.958 ms with $m$ ranging from 1 to 20. The average candidate set size on which we compute true distances ranges from $19.8K$ to $349K$ (the union of candidates across 8 nodes).
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**Lemma 1** Consider a process where we sample $K$ elements from a universe of $B$ elements without replacement, with arbitrary probabilities $p_1, p_2, ..., p_B$. Denote the score $T$ of this sample set to be the mean of the $K$ sampling probabilities. The variance of $T$ is given by

$$ \frac{1}{K^2} \sum_{i=1}^{K} p_i^2 (1 - p_i) $$

**Proof:** Suppose we are to measure a characteristic $x_i$ for the $K$ elements in the sample.

Let us define $T = \sum_{i=1}^{K} \frac{x_i}{p_i}$. Then, as shown in the theory of importance sampling (Horvitz and Thompson, 1952), we have

$$ \text{Var}(T) = T^2 - \sum_{i=1}^{K} \frac{x_i^2}{p_i} - \sum_{i \neq j} \frac{x_i x_j}{p_ip_j} $$

In this theorem, by choosing $x_i = \frac{p_i^2}{K}$, we have $T = \frac{1}{K} \sum_{i=1}^{K} p_i$ and

$$ \text{Var}(T) = \left( \frac{\sum_{i=1}^{K} p_i}{K} \right)^2 - \frac{\sum_{i=1}^{K} p_i^3}{K^2} - \frac{\sum_{i \neq j} p_ip_j}{K^2} $$

$$ \Rightarrow \text{Var}(T) = \frac{1}{K^2} \left( \sum p_i^2 - \sum p_i^3 \right) $$

$$ \Rightarrow \text{Var}(T) = \frac{1}{K^2} \left( \sum p_i^2 - \sum p_i^3 \right) $$

It is easy to see that $\text{Var}(T)$ is a monotonic decreasing function (say $f_m(K)$) of $K$ as it goes down faster than $O(1/K)$.

**Implications:** Please recall that in IRLI, for any input, we pick the top-$K$ buckets of the $B$ based on the probability scores. Hence, of all the $B$-choose-$K$ combinations, the $K$-tuple that we pick has the maximum mean of probabilities compared to every other $K$-tuple (vice versa, the $K$-tuple having the maximum mean of probabilities is also the one with all the top-$K$ buckets).

Lemma 1 shows that the variance of the mean of the probabilities of the $K$-tuple decreases with $K$.

This simulates a virtual random process of picking any tuple with equal likelihood and leads to the following theorem.

**Theorem 2:** Consider the process where at each step, a label is chosen independently and uniformly at random and is inserted into the index. Each new label $l$ inserted in the index chooses $K > K_0$ possible destination bins which are the top-$K$ indices of $P_l$, and is placed in the least full of these bins. For a sufficiently large $t$, the most crowded bin at time $t$ contains fewer than $\frac{\log(\log(L)+f_1(K))}{\log(K)} + O(1) + f_2(K)$ labels with high probability, where $f_1$ and $f_2$ are monotonically decreasing functions of $K$.

**Proof:** Let the number of bins with load $\geq i$ at the end of time $L$ (i.e., the end of the re-partitioning) to be less than $\beta_i$. Given that we know $\# \text{bins}_{\geq i}(L) \leq \beta_i$, we need to find an upper-bound $\# \text{bins}_{\geq i+1}(L)$ to find the max of bins.

In the event of a collision, consider that each label stacks up the on the existing labels like a tower. The height of a label in that case is the number of labels below it. Let $\# \text{labels}_{\geq i}(t)$ represent the number of labels that have height $\geq i$ after total $t$ insertions.

Please note that $\# \text{labels}_{\geq i}(t)$ is always larger than the $\# \text{bins}_{\geq i}(t)$, as each bin with $\geq i$ has at least one label with height $\geq i$.

For a new label to land at height $\geq i + 1$, all $K$ bins (that we pick) should have load of at least $i$. With the assumption made in (Mitzenmacher, 2001), where the $K$ bins are chosen randomly, the probability of choosing $K$ bins that have height $\geq i$ is at most

$$ p_i = \left( \frac{\beta_i}{B} \right)^K $$

Since the number of bins with $\frac{2L}{B}$ can almost be $\frac{B}{2}$, we have $\beta_{\frac{2L}{B}} \leq \frac{B}{2}$. However, we select the top $K$ bins based on the maximum affinity scores for a given query vector (instead of random $K$ bins). In this case, for any sufficiently large $K \geq K_0$, the probability $p_i$ is almost

$$ p_i \leq \left( \frac{\beta_i}{B} \right)^K + \delta $$

where $\delta$ is a monotonically decreasing function of $K$ (by
invoking Lemma 1).

\[ \delta = f_m(K) \]

Pardon the abuse of notation, please don’t confuse this with the \( \delta \) used in Theorem 1.

Hence the \( t^{th} \) label has height \( \geq i + 1 \) with probability atmost \( \rho_i \). Number of labels that have height \( \geq i + 1 \) is atmost \( L\rho_i \). For a fixed IRLI index parameters \( L > B \). We can safely assume that \( L = \frac{B}{c} \), where \( c < 1 \).

\[ \beta_{i+1} = L\rho_i = \frac{B}{c} \left( \frac{\beta_i}{B} \right)^{k} + \delta \]

Just like the case of random \( K \) selection, we can set \( \beta_{2/c} \leq B/2 + \delta \). We now find an expression for \( \beta_{2/c+1} \) using induction

\[ \beta_{2/c+1} = \frac{B}{c} \left( \frac{1}{2K} + \delta_1 \right) \]

\[ \beta_{2/c+2} = \frac{B}{c} \left( \frac{1}{2K^2 c^{K_i}} + \delta_2 \right) \]

Here each \( \delta_i \) is a positive real number, monotonically decreasing in \( K \). The \( \beta_{2/c+i} \) is given by

\[ \beta_{2/c+i} = \frac{B}{c} \left( \frac{1}{2K^i c^{K_i}} + \delta_i \right) \]

Going by the definition of \( \beta_i \), if \( \beta_i \leq 1 \), then \( i \) represents that maximum load across all the buckets. That happens when

\[ \frac{B}{c} \left( \frac{1}{2K^i c^{K_i}} + \delta_i \right) \leq 1 \]

\[ i = \log_K \left( \log \left( \frac{L}{1 - L\delta_i} \right) \right) - \log_K \left( 1 + \frac{1}{K} \log c \right) \]

This can be further simplified into

\[ i^* = \frac{2c}{c} + i = \frac{\log \left( \log L + f_1(K) \right)}{\log K} + f_2(K) + 2L/B \]

Where \( f_1(K) = -\log(1 - L\delta_i) \) and \( f_2(K) = \log_K(1 + \frac{1}{K} \log c) \). As \( \delta_i \) decreases with \( K \), \( f_1(.) \) also monotonically decreases.

And using the fact that the derivative of

\[ \frac{\log(1 + \frac{\log c}{\log x})}{\log x} \]

is negative for \( x > 1 \), we can conclude that \( f_2(.) \) is also a decreasing function of \( K \).