
Quit When You Can: Efficient Evaluation of Ensembles with Ordering Optimization

Serena Wang

Google, Inc.

serenawang@google.com

Maya Gupta

Google, Inc.

mayagupta@google.com

Seungil You

Kakao Mobility

sean.you@kakaomobility.com

Abstract

Given a classifier ensemble and a set of examples to be classified, many examples may be confidently and accurately classified after only a subset of the base models in the ensemble are evaluated. This can reduce both mean latency and CPU while maintaining the high accuracy of the original ensemble. To achieve such gains, we propose jointly optimizing a fixed evaluation order of the base models and early-stopping thresholds. Our proposed objective is a combinatorial optimization problem, but we provide a greedy algorithm that achieves a 4-approximation of the optimal solution for certain cases. For those cases, this is also the best achievable polynomial time approximation bound unless $P = NP$. Experiments on benchmark and real-world problems show that the proposed *Quit When You Can* (QWYC) algorithm can speed-up average evaluation time by 2x–4x, and is around 1.5x faster than prior work. QWYC’s joint optimization of ordering and thresholds also performed better in experiments than various fixed orderings, including gradient boosted trees’ ordering.

1 Introduction

We consider the problem of efficiently evaluating a binary classifier that can be expressed as an ensemble of T base models, $f(x) = \sum_{t=1}^T f_t(x)$, where each base model $f_t(x) \in \mathbb{R}$ contributes a score. The ensemble may have been trained:

Independently: Each f_t is trained individually, for example, random forests (Breiman, 2001).

Sequentially: Each f_t is trained taking into account fixed $f_1, f_2 \dots, f_{t-1}$, for example, boosted trees (Fernandez-Delgado et al., 2014).

Jointly: All f_t are trained together, for example, generalized additive models (Hastie and Tibshirani, 1990) or an ensemble of lattices (Canini et al., 2016).

Existing work on ensemble pruning can be generally categorized as static ensemble pruning or dynamic ensemble pruning. In traditional static ensemble pruning, the same pruned subensemble is used for all examples ((Zhou et al., 2002; Martinez-Munoz and Suarez, 2006; Margineantu and Dietterich, 1997; Tamon and Xiang, 2000), and many others). In contrast, in dynamic ensemble pruning, a different subensemble may be used to evaluate each example (Xiao et al., 2010).

The approach that we propose is dynamic: we propose to evaluate a larger subset of base models for examples that are more difficult to classify. The key idea is that if some examples are easy to classify, then such easy examples can be confidently and accurately classified after evaluating

only a few base models, but for hard examples, we may choose to evaluate the full ensemble. This adapts the computation to the difficulty of the classification problem, reducing average latency and computational resources (e.g. CPU) needed to classify. This dynamic approach is complementary to the traditional static ensemble pruning approach, as the dynamic approach can act on a pre-pruned ensemble to achieve even further average speedups on a per-example basis.

A variety of dynamic ensemble pruning strategies exist that rely on different heuristics for selecting subensembles. Woods et al. (1997) introduced the idea of selecting base models for different clusters of examples, and ordering the base models by accuracy within each cluster. Santana et al. (2006) showed that ordering base models by both accuracy and diversity can actually produce more accurate subensembles at test time. Santos et al. (2007) proposed a slightly different heuristic of choosing the most confident base models for each example. Fan et al. (2002) suggested ordering by total benefits of the base models, where total benefits may include some combination of accuracy and the classifier’s objective. The ultimate goal of these selection criteria is to achieve faster evaluation time without sacrificing too much performance compared to the full ensemble.

While ordering by total benefits, diversity, and confidence have been shown to work better than accuracy alone for achieving faster evaluation time, we aim to bypass these heuristics entirely by jointly optimizing the order with the pruning mechanism to directly improve the evaluation time objective without differing too much from the original ensemble.

Specifically, to dynamically prune the ensemble, we propose an objective that defines an optimal ordering π of the T base models and an optimal set of $2T$ corresponding early decision thresholds $\{\epsilon^+, \epsilon^-\}$ that minimize the average number of base models evaluated, while maintaining the accuracy of the full ensemble. We also propose a simple early stopping mechanism for a given example x as follows: after evaluating the r th base model, if the accumulated sum $\sum_{t=1}^r f_t(x)$ is above the r th early positive threshold ϵ_r^+ , then the example is classified as the positive class, and the evaluation is stopped early (and vice-versa for negative examples). Otherwise, the $r + 1$ th base model is evaluated.

While it is computationally challenging to find a globally optimal solution for this combinatorial optimization problem, we propose a greedy algorithm which we refer to as *Quit When You Can* (QWYC). For certain ensembles, QWYC achieves a 4-approximation of the optimal solution, which is also the best approximation bound that can be achieved in polynomial time unless $P = NP$. While we present QWYC with simple early stopping criteria using thresholds, other pruning mechanisms may be substituted into the QWYC algorithm to be optimized with the ordering.

Experiments on both real-world and benchmark problems show that QWYC can speed up computation time by 2x–4x while classifying faithfully compared to the full ensemble on held-out examples. QWYC’s joint optimization of ordering and early stopping criteria also performed better in experiments than various fixed heuristic orderings, including the natural ordering produced during training of gradient boosted trees (Section 5).

Our main contribution is to demonstrate both the value and practicality of jointly optimizing ordering with early stopping criteria for dynamic ensemble pruning.

2 Related Work

The most related prior work is the dynamic ensemble pruning strategy of Fan et al. (2002). The authors order the base models based on their individual utility. For example, they order from the base model that has the highest accuracy when used by itself to the base model that has the lowest accuracy when used by itself. They propose an early stopping criteria where the threshold to declare an early positive or negative class depends on a probabilistic modeling of the running score. A more detailed explanation and implementation is given in Section C. In contrast, we take a discriminative approach: we propose to jointly optimize the ordering with the early stopping criteria to minimize the expected evaluation cost, constrained to producing the same classification decisions as the full classifier within a given error margin.

One common approach in dynamic ensemble pruning involves using clustering to match examples to their most accurate subensembles. These methods require the user to specify an ordering criteria for each cluster (Woods et al., 1997). Some work has been done on improving the ordering of base models for each cluster by selecting for both accuracy and diversity instead of just accuracy

(Santana et al., 2006; Xiao et al., 2010). Our method is thus complementary to these clustering approaches – for examples in each cluster, QWYC can choose an ordering that directly reduces evaluation time rather than relying on the user to specify selection heuristics.

A special case of the efficient ensemble evaluation problem is when the base models are assumed to be independently-trained and randomly-ordered, and each base model only contributes a vote of yes or no for each class, rather than a score. Then the incomplete votes can be modeled as draws from a multinomial distribution (Hernandez-Lobato et al., 2009; Schwing et al., 2011) and the class priors can be incorporated (Soto et al., 2016). Other researchers have shown similar results using a Gaussian approximation (Basilico et al., 2011). In those papers, only intermediate thresholds for stopping early are chosen; the base models are not re-ordered as part of the speed-up.

A related but different problem is trying to adaptively minimize the set of features needed to evaluate each x , either to reduce costs or time associated with obtaining those features (Parrish et al., 2013; Wang et al., 2015; Nan et al., 2016). In this paper, we do not explicitly model feature computation at all. We depend only on the cost of evaluating each base model and treat each base model evaluation cost as independent of the cost of evaluating other base models. One could model feature evaluation costs via the base model evaluation cost, but if two base models use the same expensive feature, then our model would not take into account that the second use of the feature was essentially free.

A more general version of the problem than what we tackle here is that instead of using the same optimized ordering of the base models for all examples, one could adaptively change the choice of which base model to evaluate next (Gao and Koller, 2011; Xu et al., 2013). Such instance-adaptive orderings could potentially offer even greater gains if some of the base models are relatively expensive to evaluate. However, these orderings would require substantially greater system complexity in practice.

Others have focused on how to design and train a cascade of base models to enable significant early rejections (Viola and Jones, 2001; Li et al., 2002; Saberian and Vasconcelos, 2010). For example, Viola and Jones (2001) produced a seminal real-time face recognition systems by hand-designing a simple-to-complex cascade of classifiers that could perform early rejection. In this paper, we take the ensemble as given, and propose a method for speeding up a given already-trained ensemble.

Lastly, another strategy for fast evaluation of ensembles is to evaluate the base models in parallel. However, parallelization does not reduce the mean computational resources needed to classify, which is one of the goals of this work. Moreover, parallelized evaluation is a complementary strategy: one can parallelize sub-ensembles of base models such that each f_t represents one sub-ensemble. In practice, if one can evaluate batches of samples at a time, we have found it is less complex in terms of software engineering and more efficient to simply parallelize over samples, rather than parallelizing over base models.

3 Optimization Problem

We take as given a linearly-separable model $f(x) : x \in \mathbb{R}^D \rightarrow \mathbb{R}$ where $f(x) = \sum_{t=1}^T f_t(x)$, an expected time (or other cost) $c_t \in \mathbb{R}^+$ to evaluate the t th base model $f_t(x)$ for $t = 1, \dots, T$, and a decision threshold $\beta \in \mathbb{R}$ for classifying $f(x)$.

We propose optimizing a fast classifier over the set of all permutations of Π that map $\{1, 2, \dots, T\} \rightarrow \{1, 2, \dots, T\}$, and positive and negative threshold vectors $\epsilon^+, \epsilon^- \in \mathbb{R}^T$ to minimize the expected evaluation cost for a random sample $X \in \mathbb{R}^D$ drawn from a data distribution \mathbb{P}_X subject to $\epsilon^- \leq_+ \epsilon^+$ (here, \leq_+ is the element-wise inequality), with a constraint on what percent of samples can be classified differently by the fast classifier from the full classifier $f(x)$ controlled by a misclassification rate α :

$$\underset{\pi \in \Pi, \epsilon^- \in \mathbb{R}^T, \epsilon^+ \in \mathbb{R}^T}{\text{minimize}} \quad \mathbb{E}_X \left[\sum_{t=1}^T c_{\pi(t)} I_{X,t,\pi,\epsilon^+, \epsilon^-} \right] \quad \text{subject to } \mathbb{E}_X [Z_{X,\pi,\epsilon^+, \epsilon^-}] \leq \alpha, \quad (1)$$

$$\epsilon^- \leq_+ \epsilon^+$$

where $I_{X,t,\pi,\epsilon^+, \epsilon^-}$ is a Bernoulli random variable that is 1 if X is not classified yet after t base models in the ordering denoted by permutation π according to the decision threshold vectors ϵ^+ and ϵ^- , and is 0 otherwise; and $Z_{X,\pi,\epsilon^+, \epsilon^-}$ is a Bernoulli random variable that is 1 if the fast

classification of X differs from the full evaluation classifier decision for X , and 0 if the fast and complete classification decisions agree.

3.1 Empirical Approximation

In practice, we do not have direct access to \mathbb{P}_X and instead we take as given a set of n examples $\{x_i\}$ assumed to be sampled independently and identically from \mathbb{P}_X . Let $g_r(x, \pi)$ denote the accumulated sum (incomplete score) after r base models ordered as per π : $g_r(x, \pi) = \sum_{t=1}^r f_{\pi(t)}(x)$.

After evaluating the r th base model, an example x belongs to one of three classes—positive, negative, or uncertain: $P_r := \{x | g_r(x, \pi) > \epsilon_r^+\}$, $N_r := \{x | g_r(x, \pi) < \epsilon_r^-\}$, $U_r := \{x | \epsilon_r^- \leq g_r(x, \pi) \leq \epsilon_r^+\}$ for $r \in \{1, \dots, T\}$ and $U_0 = \mathbb{R}^D$. If $x \in P_r$ or $x \in N_r$, then x is classified as a positive or negative class, respectively, and we terminate the evaluation at the r th step. On the other hand, if $x \in U_r$, the classification decision is uncertain, and we continue to evaluate the $\pi(r+1)$ th base model. Define three more classes: $N_{\text{full}} := \{x | f(x) < \beta\}$, $P_{\text{full}} := \{x | f(x) \geq \beta\}$, $C_r := \bigcap_{t=0}^r U_t$ where C_r is the set of samples that remain unclassified after evaluating the r th base model.

We approximate the objective (1) with the empirical analogue:

$$\begin{aligned} & \underset{\pi \in \Pi, \epsilon^- \in \mathbb{R}^T, \epsilon^+ \in \mathbb{R}^T}{\text{minimize}} \quad \frac{1}{N} \sum_{t=1}^T c_{\pi(t)} \sum_{i=1}^N \mathbf{1}[x_i \in C_{t-1}] \\ & \text{subject to} \quad \frac{1}{N} \sum_{i=1}^N \mathbf{1}[x_i \in \bigcup_{t=1}^T \{C_{t-1} \cap P_t \cap N_{\text{full}}\}] \\ & \quad + \frac{1}{N} \sum_{i=1}^N \mathbf{1}[x_i \in \bigcup_{t=1}^T \{C_{t-1} \cap N_t \cap P_{\text{full}}\}] \leq \alpha \text{ and } \epsilon^- \leq_+ \epsilon^+. \end{aligned} \tag{2}$$

In Section 4, we give an algorithm to approximately optimize (2).

Representative Dataset: Certainly the value of the solution to (2) will depend on how representative the examples $\{x_i\}$ are of the examples that will be seen in actual usage of the model. Because optimizing (2) does not require labels for the examples, it is often easier in practice to obtain a large number of unlabeled examples to use in optimizing (2).

Filtering Candidates: An important use case in practice for fast classification is when the prior probability is for the negative class, and we wish to reject examples quickly. For example, when recommending products to a user from a database of millions of products, one hopes to quickly reject most products, but the most promising ones should be fully-scored, and then their classifier scores can be sorted to rank the remaining small set of top candidates. For such cases, the objective (2) can be simplified to only finding early-rejection thresholds $\{\epsilon_t^-\}$, as any positively classified samples will need the full score and must thus be fully evaluated.

4 QWYC: Optimizing the Order and Early-Stopping Thresholds

Since (2) is a combinatorial optimization over π , coupled with $2T$ -dimensional optimization over the real-valued threshold vectors ϵ^- and ϵ^+ , we have little hope of finding a global optimum except for small T . We propose a greedy optimization of (2) for both the ordering of the base models and the thresholds, which we refer to as *Quit When You Can* (QWYC).

The greedy optimization proceeds iteratively, first calculating the optimal thresholds to satisfy the constraints of (2) for each of the possible T base models that could be selected as the first base model $\pi(1)$. The base model that minimizes the evaluation time ratio is then set as $\pi(1)$ with its corresponding optimized thresholds. The process is then repeated for each of the base models in order, taking into account the previous chosen base models and thresholds. The evaluation time ratio J_t is defined as

$$J_t(\epsilon^+, \epsilon^-, \pi) = \frac{c_{\pi(t)} \sum_{i=1}^N \mathbf{1}[x_i \in C_{t-1}]}{n_{\pi(t)}}$$

where $n_{\pi(t)} = \sum_{i=1}^N \mathbf{1}[x_i \in C_{t-1} - C_t]$ is the number of additional examples for which submodel $\pi(t)$ is able to stop evaluating early. Intuitively, J_t is the additional evaluation time required to stop evaluating early on each example.

Algorithm 1 details this procedure, where we have pulled out the QWYC optimization of the thresholds into a subroutine detailed in Algorithm 2. Optimizing (2) for each ϵ_r^- can be done using binary search, since the objective is monotonically decreasing with respect to ϵ_r^- , and the constraint is monotonically increasing with respect to ϵ_r^- (and analogous logic holds for each ϵ_r^+). Assuming that the binary search is $O(N)$ where N is the size of the dataset (given a limited number of iterations), the time complexity for this procedure is $O(T^2 N)$. The QWYC early-stopping thresholds can be computed for any ordering of the base models, and in the experiments we compare different ordering methods combined with QWYC early stopping thresholds.

Algorithm 1 Optimize Order

```

1: Initialize  $\pi(i) \leftarrow i$  for  $i = 1, \dots, T$ 
2: for  $r = 1$  to  $T$  do
3:   Initialize  $k^* \leftarrow r$ 
4:   Initialize  $J_r^* \leftarrow \infty$ 
5:    $\epsilon_r^{+*} \leftarrow \infty, \epsilon_r^{-*} \leftarrow -\infty$ 
6:   for  $k = r$  to  $T$  do
7:     Swap  $\pi(r)$  with  $\pi(k)$ 
8:      $\epsilon_r^{+'}, \epsilon_r^{-'} \leftarrow \text{Optimize Thresholds}(\pi, \epsilon^+, \epsilon^-)$ 
9:     if  $J_r(\pi, \epsilon^+, \epsilon^-) < J_r^*$  then
10:       $J_r^* \leftarrow J_r(\pi, \epsilon^+, \epsilon^-)$ 
11:       $\epsilon_r^{+*} \leftarrow \epsilon_r^{+'}, \epsilon_r^{-*} \leftarrow \epsilon_r^{-'}$ 
12:       $k^* \leftarrow k$ 
13:    end if
14:    Swap  $\pi(r)$  with  $\pi(k)$                                  $\triangleright$  Revert  $\pi$ 
15:  end for
16:  Swap  $\pi(r)$  with  $\pi(k^*)$ ,  $\epsilon_r^+ \leftarrow \epsilon_r^{+*}, \epsilon_r^- \leftarrow \epsilon_r^{-*}$ 
17: end for
18: return  $\pi, \epsilon^+, \epsilon^-$ 

```

Algorithm 2 Optimize Thresholds

```

1: Input: Index  $r$  to optimize
2: Input:  $\epsilon_1^-, \epsilon_2^-, \dots, \epsilon_{r-1}^-$  and  $\epsilon_1^+, \epsilon_2^+, \dots, \epsilon_{r-1}^+$ 
3: Input:  $\pi(1), \pi(2), \dots, \pi(r)$ 
4: Optimize (2) with  $T = r$  for  $\epsilon_r^-$  using binary search.
5: Optimize (2) with  $T = r$  for  $\epsilon_r^+$  using binary search.
6: return  $\epsilon_r^+, \epsilon_r^-$ 

```

4.1 QWYC Approximation Bound

In certain cases, the problem of finding the optimal ordering and early stopping thresholds reduces to the Pipelined Set Cover problem (Munagala et al., 2005), and the QWYC greedy algorithm therefore achieves a 4-approximation of the optimal evaluation time.

Let $S_t(i)$ be the maximal set of examples for which base model f_t can make an early negative or early positive classification while satisfying the constraint when $\alpha = 0$ and $\pi(i) = t$ after a binary search over $\epsilon_i^+, \epsilon_i^-$ (assuming no early stopping before reaching the i th base model). For $i \geq 1$, $S_t(i) \supseteq S_t(1)$. Depending on the base models that came before the i th base model, $S_t(i)$ may contain more elements than $S_t(1)$. Let OPT be the optimal cost under the conservative restriction that $S_t(i) = S_t(1)$ for $i \geq 1$. Let OPT^* be the true optimal cost. Define PIPELINE to be the set of problems where $OPT \leq OPT^* + C$, such that the optimal cost that restricts early stopping to $S_t(1)$ differs by a constant from the true optimal cost. While this constant may seem arbitrary, we provide a concrete example of a problem from PIPELINE in Appendix A.1.

Theorem 1. *For problems in PIPELINE, the QWYC algorithm achieves a 4-approximation of the optimal cost, which is also the best achievable approximation bound unless $P = NP$.*

Proof. In Appendix A. □

5 Experiments

We demonstrate the performance of QWYC’s joint optimization of ordering and early stopping thresholds on four datasets detailed in Table 1 (in Appendix): two benchmark datasets, and two real-world case studies from a large internet services company. For datasets without a pre-defined train/test split, we randomly shuffle the dataset and split it 80-20 to produce a train and test set. The train set is used to optimize the ordering and early stopping thresholds.

Let QWYC* refer to Algorithm 1, our proposed joint optimization of ordering and early stopping thresholds. To illustrate the effectiveness this joint optimization, we compare QWYC* to the baseline of fixing a variety of pre-selected orderings while optimizing the early stopping thresholds using Algorithm 2. We describe these pre-selected orderings in Appendix B.

We also compare QWYC* to the suggested ordering and early stopping mechanism proposed by Fan et al. (2002). Fan et al. (2002) suggest pre-selecting an ordering by individual total benefits, and propose an early stopping mechanism that is more complex and flexible than Algorithm 2. We describe their early stopping mechanism in detail in Appendix C. They use Individual MSE as a simple total benefits metric. Let Fan* refer to the early stopping mechanism of Fan et al. (2002) with pre-selected Individual MSE ordering. In addition to Individual MSE, for every pre-selected ordering we try with Algorithm 2, we also try it with the Fan et al. (2002) early stopping mechanism.

Overall, we compare QWYC*’s joint optimization of ordering and thresholds to:

1. Fan*: the suggested ordering and early stopping method of Fan et al. (2002).
2. Combining different pre-selected orderings with our simple early stopping thresholds (Algorithm 2) and the more flexible early stopping mechanism proposed by Fan et al. (2002).
3. Training a smaller ensemble, but always fully evaluating it.

To illustrate the tradeoff between fast evaluation and faithfulness to the full ensemble, we vary the α hyperparameter that controls the maximum % classification differences from the full ensemble for experiments that use either the QWYC* joint optimization or Algorithm 2 with other pre-selected orderings. Similarly, for comparisons that use the Fan et al. (2002) early stopping mechanism, we vary the γ hyperparameter that indirectly controls the % classification differences from the full ensemble.

Benchmark Experiments Set-up: For the Adult and the Nomao benchmark datasets from the UCI Machine Learning Repository (Lichman, 2013), we train gradient boosted tree (GBT) ensemble models (Friedman, 2001). A GBT ensemble model is an additive model where the output is the sum of T regression trees. The training process produces a natural ordering of the trees because each tree is added to the ensemble sequentially, which we compare to in experiments. When training the full ensemble, we perform hyperparameter optimization on a validation set over the number of base trees in the ensemble, the maximum depth of a single base tree, and the learning rate. We treat the evaluation cost of each base model as a constant $c_t = 1$ for all t , which is a conservative assumption as the maximum depth of each base tree is bounded.

Experiment 1: UCI Adult Dataset: This is a binary classification task where the objective is to predict whether or not a person’s income is greater than \$50,000. The full ensemble has $T = 500$ base trees of maximum depth 5 and acts on a total of $D = 14$ features. We use the predefined train/test split provided in the repository.

Experiment 2: UCI Nomao Dataset: This is a binary classification task where the goal is dedduplication: each labeled example contains information about 2 sources, and the label denotes whether those 2 sources refer to the same business. The full ensemble has $T = 500$ base trees of max depth 9 and uses the strongest $D = 8$ features out of 120 available features.

We compare the performance of QWYC* to the Fan et al. (2002) early stopping method with their suggested pre-selected ordering by Individual MSE. We also compare QWYC* to a baseline of training smaller gradient boosted tree ensembles. Finally, since gradient boosted trees produce a

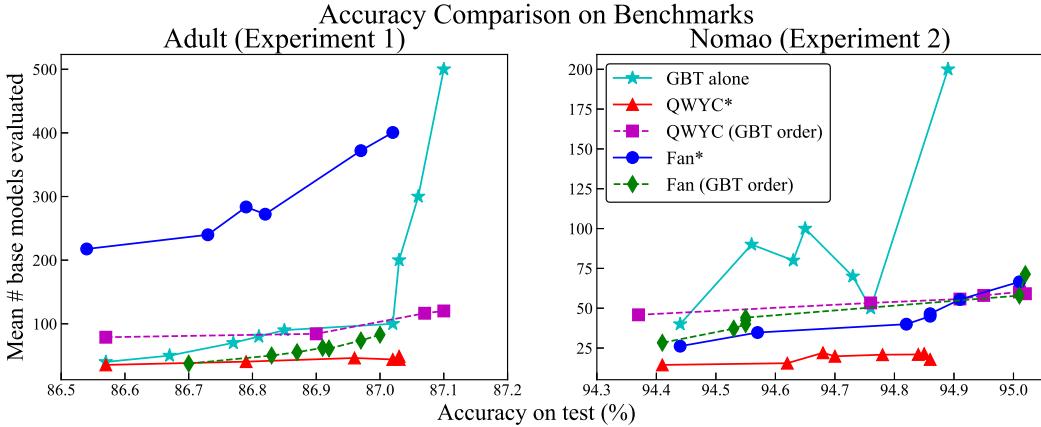


Figure 1: Test accuracy vs. mean # base models evaluated for Adult and Nomao experiments. QWYC (GBT order) refers to Algorithm 2 with pre-selected GBT ordering, and Fan (GBT order) refers to Fan et al. (2002) early stopping mechanism with pre-selected GBT ordering.

natural ordering of base models in the training process, we compare to the additional baseline of using the original gradient boosted tree ordering as a pre-selected ordering. Figure 1 shows the tradeoff between accuracy and the number of base models evaluated for QWYC*, Fan*, and these baselines.

Real-World Experiments Set-up: The two real-world case studies from a large internet services company are both Filter-and-Score problems: the goal is to quickly filter the negative examples, and if the algorithm makes a positive classification then the full ensemble $f(x)$ is required for further processing by later stages. Thus, only ϵ^- is optimized. Note that the fact that the sizes of the train and test datasets are fairly small (see Table 1) is not indicative of the need for fast evaluation. For example, real-world case study 1 requires evaluating the model over one trillion examples a day in response to real-time requests.

For the real-world case studies, we were given ensemble models where the base models are lattices, which are interpolated look-up tables (LUTs), and can be trained with the open-source package TensorFlow Lattice (Canini et al., 2016). See Appendix D.1 for more details on lattice ensembles. We were given jointly-trained ensembles, but we re-trained each ensemble with independent-training of the base models to be able to compare speed-ups for independently-trained vs jointly-trained.

Experiment 3: Real-World 1, Jointly Trained: For this Filter-and-Score problem, the full ensemble contains $T = 5$ jointly trained base models, and each base model acts on 13 features out of a total set of $D = 16$ features, where the feature subsets for the 5 base models are chosen to maximize the interactions of the features in each base model as per Canini et al. (2016). The train dataset has 183,755 examples and the test dataset has 45,940. The task is heavily biased to rejecting candidates: a priori, the probability a sample will be classified negative by the full ensemble is 0.95.

Experiment 4: Real-World 2, Jointly Trained: For this Filter-and-Score problem, the full ensemble contains $T = 500$ jointly trained base models, each base model acted on 8 features out of a total set of $D = 30$ features, and the 500 feature subsets were randomly generated, which means that some base models can be expected to be much more useful than others. The train dataset has 83,817 examples and the test dataset has 20,955. The class priors are roughly equal.

Experiments 5 and 6 performed on independently-trained ensembles are detailed in Appendix D.3.

An important difference between the real-world datasets and the benchmark datasets is that the real-world held-out evaluation sets do not always contain the training label, so we do not report accuracies for real-world experiments. This illustrates an important advantage of QWYC*: QWYC* does not require labeled data to optimize for evaluation time, and in production systems, it is often easier to collect unlabeled data that matches the true test distributions than labeled data.

Figure 2 shows the tradeoff between % classification differences and mean # base models evaluated for Experiments 3-6. Since these models are productionized, we also report timing numbers for

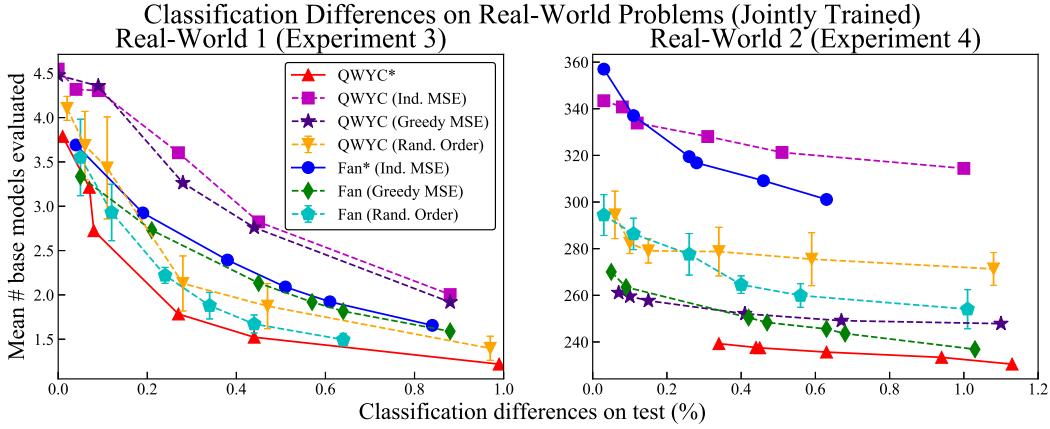


Figure 2: Classification differences vs. mean # base models evaluated for real-world experiments with jointly trained ensembles. The error bars for Random Order show the standard deviation after 5 trials with different random orderings.

QWYC* and Fan* at $\approx 0.5\%$ classification differences in Tables 2 and 3 in Appendix D. This amount of allowed difference was chosen based on a rough estimate of the percent of examples for which the ground truth label is likely noisy. We report the mean and standard deviation of the per-example evaluation time on the test set after 100 runs.

Discussion: In Experiments 1-5, QWYC*'s joint optimization of ordering and early stopping thresholds outperformed any pre-selected ordering combined with Algorithm 2 or Fan et al. (2002) early stopping mechanisms in terms of tradeoffs between # base models evaluated and % classification differences and accuracy (Figures 1, 2, 3 and 4). In Experiment 6, Random Order outperformed all orderings including QWYC*, and we suspect that this is because for an independently trained ensemble of 500 base models where the base models behave very similarly, a random order is less likely to overfit on a training set than a more “clever” ordering like Individual MSE, Greedy MSE, or QWYC*.

Timing experiments on both real world case studies show faster mean evaluation speeds from QWYC* than Fan*, ranging from 1.8x speed-up for the independently-trained ensemble of $T = 5$ base models in Table 4, to a notable 4x speed-up for the jointly-trained ensemble of $T = 5$ base models in Table 3.

In Experiment 1, Fan* performed worse than the baseline of smaller ensembles alone in terms of accuracy and classification differences. We suspect that this is because the Individual MSE ordering did not adequately capture a good cumulative ordering in Experiment 1. We see a similar effect in Experiments 3-6 when the gap between Individual MSE and Greedy MSE is more pronounced with jointly-trained ensembles than independently-trained ensembles.

For many pre-selected orderings, the Fan et al. (2002) early stopping mechanism performed better than the simple early stopping mechanism in Algorithm 2. Note that the Fan et al. (2002) early stopping mechanism is significantly more flexible than Algorithm 2, with at least 20 thresholds per base model (2 thresholds per bin) rather than just 2 thresholds per base model. This suggests that the QWYC optimization may achieve even better reductions in number of base models if combined with the more flexible early stopping thresholds of Fan et al. (2002). However, adding these thresholds increases model complexity and also adds its own evaluation time cost. Even with the simpler early stopping thresholds, QWYC*'s joint optimization of orderings and thresholds was both faster and more accurate than the Fan et al. (2002) early stopping criteria combined with any pre-selected orderings, which suggests that the joint optimization of ordering and early stopping criteria is valuable.

6 Conclusions and Open Questions

We provide the QWYC algorithm, which makes it possible to approximately solve the combinatorial joint optimization of ordering with an early stopping mechanism in practice. QWYC achieves the best approximation bound in polynomial time for certain cases. We have shown experimentally that QWYC's joint optimization of ordering with an early stopping mechanism can produce better results than various pre-selected ordering choices, even when those orderings are combined with more flexible early stopping criteria. While we focused here on binary classification, it is straightforward to extend the proposed optimization strategy to multi-class classifiers. Whether a similar strategy can be effectively devised for ranking or regression is an open question. While we use a simple early stopping mechanism based on thresholds in our experiments, other pruning mechanisms may be substituted into the QWYC algorithm, and our main contribution is to demonstrate that such joint optimization of the ordering and early stopping mechanism is both valuable and practical.

References

- J. D. Basilico, M. A. Munson, T. G. Kolda, K. R. Dixon, and W. P. Kegelmeyer. COMET: a recipe for learning and using large ensembles on massive data. *Intl. Conf. Data Mining (ICDM)*, 2011.
- L. Breiman. Random forests. *Machine Learning*, 45(1):5–32, 2001.
- K. Canini, A. Cotter, M. M. Fard, M. R. Gupta, and J. Pfeifer. Fast and flexible monotonic functions with ensembles of lattices. *Advances in Neural Information Processing Systems (NIPS)*, 2016.
- W. Fan, F. Chu, H. Wang, and P. S. Yu. Pruning and dynamic scheduling of cost-sensitive ensembles. *AAAI*, 2002.
- U. Feige, L. Lovasz, and P. Tetali. Approximating min-sum set cover. *Algorithmica*, 2004.
- M. Fernandez-Delgado, E. Cernadas, S. Barro, and D. Amorim. Do we need hundreds of classifiers to solve real world classification problems? *Journal Machine Learning Research*, 2014.
- J. Friedman. Greedy function approximation: a gradient boosting machine. *Annals of Statistics*, 29: 1189–1232, 2001.
- T. Gao and D. Koller. Active classification based on value of classifier. *Advances in Neural Information Processing Systems (NIPS)*, 2011.
- T. Hastie and R. Tibshirani. *Generalized Additive Models*. Chapman Hall, New York, 1990.
- D. Hernandez-Lobato, G. Martinez-Munoz, and A. Suarez. Statistical instance-based pruning in ensembles of independent classifiers. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 31(2):364–369, 2009.
- S. Z. Li, Z. Q. Zhang, H. Shum, and H. J. Zhang. Floatboost learning for classification. *Advances in Neural Information Processing Systems (NIPS)*, 2002.
- M. Lichman. UCI machine learning repository, 2013. URL <http://archive.ics.uci.edu/ml>.
- D. Margineantu and T. Dietterich. Pruning adaptive boosting. *Proc. Intl. Conf. on Machine Learning (ICML)*, 1997.
- G. Martinez-Munoz and A. Suarez. Pruning in ordered bagging ensembles. *Proc. Intl. Conf. on Machine Learning (ICML)*, 2006.
- K. Munagala, S. Babu, R. Motwani, and J. Widom. The pipelined set cover problem. *International Conference on Database Theory*, 2005.
- F. Nan, J. Wang, and V. Saligrama. Pruning random forests for prediction on a budget. *Advances in Neural Information Processing Systems (NIPS)*, 2016.
- N. Parrish, H. Anderson, M. R. Gupta, and D. Y. Hsiao. Classifying with confidence from incomplete information. *Journal Machine Learning Research*, 2013.
- M. J. Saberian and N. Vasconcelos. Boosting classifier cascades. *Advances in Neural Information Processing Systems (NIPS)*, 2010.
- A. Santana, R. Soares, A. Canuto, and M. Souto. A dynamic classifier selection method to build ensembles using accuracy and diversity. *Proceedings of the Ninth Brazilian Symposium on Neural Networks (SBRN)*, pages 36–41, 2006.
- E. Santos, R. Sabourin, and P. Maupin. Ambiguity-guided dynamic selection of ensemble of classifiers. *Proceedings of International Conference on Information Fusion*, 2007.
- G. A. Schwing, C. Zach, Y. Zheng, and M. Pollefeys. Adaptive random forest - how many experts to ask before making a decision? *CVPR*, 2011.
- V. Soto, A. Suarez, and G. Martinez-Munoz. An urn model for majority voting in classification ensembles. *Advances in Neural Information Processing Systems (NIPS)*, 2016.

- C. Tamon and J. Xiang. On the boosting pruning problem. *Proc. 11th European Conference on Machine Learning (ECML)*, 2000.
- P. Viola and M. Jones. Robust real time object detection. *ICCV Workshop on Statistical and Computational Theories of Vision*, 2001.
- J. Wang, K. Trapeznikov, and V. Saligrama. Efficient learning by directed acyclic graph for resource constrained prediction. *Advances in Neural Information Processing Systems (NIPS)*, 2015.
- K. Woods, W. Kegelmeyer, and K. Bowyer. Combination of multiple classifiers using local accuracy estimates. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 19:405–410, 1997.
- J. Xiao, C. He, X. Jiang, and D. Liu. A dynamic classifier ensemble selection approach for noise data. *Information Sciences*, 180:3402–3421, 2010.
- Z. Xu, M. J. Kusner, K. Q. Weinberger, and M. Chen. Cost-sensitive tree of classifiers. *ICML*, 2013.
- Z. Zhou, J. Wu, and W. Tang. Ensembling neural networks: many could be better than all. *Artificial Intelligence*, 137:239–263, 2002.

A Proofs

Theorem 1. *For problems in PIPELINE, the QWYC algorithm achieves a 4-approximation of the optimal cost, which is also the best achievable approximation bound unless $P = NP$.*

Proof. Let $\alpha = 0$ and restrict $S_t(i) = S_t(1)$ regardless of position i . Let OPT be the evaluation time cost of the optimal ordering and thresholds under these restrictions. Finding the optimal $\pi, \epsilon^+, \epsilon^-$ under these restrictions then maps directly onto the Pipelined Set Cover problem, where the goal is to find the optimal ordering π such that the ordered sequence of sets $S_{\pi(1)}(1), \dots, S_{\pi(T)}(1)$ covers all possible training examples contained in $\cup_{t=1}^T S_t(1)$ while achieving the lowest total evaluation time cost.

Theorem 1 by Munagala et al. (2005) shows that the Greedy algorithm that chooses the set that minimizes the cost ratio each time achieves a 4-approximation of OPT . Since QWYC minimizes the evaluation time ratio J_r when choosing the r th base model and early stopping thresholds ϵ_r^+ and ϵ_r^- , QWYC achieves a 4-approximation of OPT .

Since in PIPELINE, $OPT \leq OPT^* + C$, QWYC also achieves a 4-approximation of OPT^* for problems in PIPELINE.

Feige et al. (2004) also show that problems in PIPELINE with uniform cost do not admit to better than a 4 approximation unless $P = NP$. \square

A.1 Example of a problem in PIPELINE

Let $\alpha = 0$ and let $c_t = 1$ for all t . Suppose there are examples $\{e_1, \dots, e_8\}$ and base models f_1, f_2, f_3 , and the decision threshold is 0 for the full classifier $\sum_{t=1}^3 f_t$. Let the individual classification decisions for f_1, f_2, f_3 be as follows:

$$\begin{aligned} f_1(e_1) &= 1, f_1(e_2) = -1 \text{ and } 0 \text{ for all others,} \\ f_2(e_3) &= 1, f_2(e_4) = 1, f_2(e_5) = -1 \text{ and } 0 \text{ for all others, and} \\ f_3(e_5) &= -1, f_3(e_6) = 1, f_3(e_7) = -1, f_3(e_8) = -1 \text{ and } 0 \text{ for all others.} \end{aligned}$$

For this problem, $S_1(i) = S_1(1) = \{e_1, e_2\}$ regardless of where f_1 is evaluated with respect to f_2 and f_3 . The same is true for $S_2(i)$ and $S_3(i)$. Thus, the optimal order is $\pi = [3, 2, 1]$ and the optimal evaluation time cost is $OPT = OPT^* = \frac{1}{8}(8c_3 + 4c_2 + 2c_1) = \frac{7}{4}$.

B Comparison of Different Orderings

To illustrate the effectiveness of QWYC*'s joint optimization of ordering and early stopping thresholds in Algorithm 1, we compare QWYC* to baselines where we combine Algorithm 2 with pre-specified orderings. For completeness of evaluating these orderings, we also compare to hybridized versions of the Fan et al. (2002) proposal that mixes their early stopping mechanism with other pre-specified orderings. We describe all pre-selected orderings that we use in experiments here:

Gradient Boosted Tree (GBT) Ordering: GBT ensembles are trained in a greedily additive fashion, where each base regression tree f_t is selected to be the one that most improves the training objective when added to the subensemble of size $t - 1$. Thus, this training procedure produces a natural ordering of base trees that we compare to.

Random Ordering: Random ordering of the base models is a random permutation drawn uniformly from all possible permutations of $\{1, \dots, T\}$. In each experiment, we report the mean and standard deviation of results across 5 random permutations.

Order by Individual MSE: As done by Fan et al. (2002), one can choose the ordering of the base models π based on each base model's individual accuracy or MSE, if one has access to labeled examples. For other precision-recall trade-offs, the best individual ordering may be slightly different. In preliminary experiments, we found ordering by the models' individual MSE's to be more useful than ordering by their training accuracies.

Order by Greedy MSE: Ordering by individual MSE can cause many highly-correlated very-accurate classifiers to all be ordered first. Theoretically, a more optimal strategy is to first choose the best individual model (by MSE), and then greedily choose each subsequent base model

to minimize the MSE of the partial ensemble. This type of greedy ordering is similar to the gradient boosted tree ordering and to other approaches used in non-dynamic ensemble pruning (Martinez-Munoz and Suarez, 2006).

C Details on the Early Stopping Criteria by Fan et al. (2002)

We compare to the dynamic ensemble pruning strategy proposed by Fan et al. that they refer to as *dynamic scheduling* (Fan et al., 2002). Fan et al. recommend that the base models be ordered by decreasing total benefits, where total benefits is suggested to be the mean squared error (MSE) of the individual base model. We refer to this ordering as Individual MSE.

For a given order of the base models, Fan et al. choose multiple thresholds per base model, one per bin of incomplete scores (Fan et al., 2002). They originally apply their method to averaging ensembles, but it is straightforward to extend their method without modification to additive ensembles. For clarity, we describe our implementation of this in some detail.

Let $g_r(x) = \sum_{t=1}^r f_t(x)$ denote the partial ensemble evaluation up through base model r . Let β be the decision threshold for classifying the full ensemble evaluation $f(x) = \sum_{t=1}^T f_t(x)$.

For each base model r , define a distinct set \mathcal{B}_r of bins into which $g_r(x)$ will be mapped, and let $b_r(x) \in \mathcal{B}$ denote the bin that $g_r(x)$ is assigned to.

For every bin $B_r \in \mathcal{B}_r$, let $\mu_{B_r}, \sigma_{B_r}^2$ denote the empirical mean and variance of the differences compared to the full ensemble evaluation for a set of representative examples that are mapped to B_r . Let γ be a confidence hyperparameter that is set by the user to control the accuracy of the early stopping with respect to the full ensemble evaluation. Then the early stopping thresholds after the r th base model evaluation and the bin B_r are:

$$\epsilon_{r,B_r}^+ = \mu_{B_r} + \gamma\sigma_{B_r} \quad \text{and} \quad \epsilon_{r,B_r}^- = \mu_{B_r} - \gamma\sigma_{B_r}.$$

Fan et al. does not specify a concrete method for how to map $g_r(x)$ to a bin. We found the best and most efficient results using rounding and a knob λ to control how many bins there are: bin $g_r(x)$ as $b_r(x) = \text{floor}(g_r(x)/\lambda)$, and note $b_r(x)$ is then some $B_r \in \mathcal{B}_r$. As recommended by Fan et al., we map the bin values to confidence parameters using a hash table to save evaluation time. For all experiments, we vary the knob λ between 0.1 and 0.001 to test more or fewer bins, causing the mean number of bins per base model to range from 10 to 400. If one uses a large number of bins (small λ) we found too few training examples fell into each bin and led to high generalization error, and that a value of $\lambda = 0.01$ produced the best tradeoff between speed and accuracy for most experiments.

Thus the decision rule for each example x after the r th base model evalution is:

$$\begin{cases} g_r(x) > \beta + \epsilon_{r,b_r(x)}^+, & \text{classify positive} \\ g_r(x) < \beta + \epsilon_{r,b_r(x)}^-, & \text{classify negative} \\ \text{otherwise} & \text{continue evaluating.} \end{cases}$$

It can happen that during evaluation time, an example x is mapped to a bin that does not exist in the hash table if no examples were mapped to that bin on a train set. In that case, Fan et al. (2002) say to perform the full evaluation for x , which is what we do in such cases. In our experiments this happened only for around 10 examples.

D Additional Experimental Results and Discussion

D.1 Description of Lattice Ensembles

For the real-world experiments, we were given ensembles of Lattices. Lattices are similar in evaluation time and flexibility to decision trees, but have the advantages that they produce continuous real-valued outputs $f_t(x) \in \mathbb{R}$, and result in overall ensemble function $f(x)$ that is smooth and continuous, rather than piecewise-constant (Canini et al., 2016). The evaluation time for each lattice base model will be roughly equal across an ensemble (since each lattice acts on the same number of features), so we model the base model evaluation costs as $c_t = 1$ for all t .

Table 1: Datasets and Ensembles Used in Experiments

Dataset	# Feat.	Train	Test	Ens. type	Ens. size	Early Stopping
UCI Adult	14	32,561	16,281	Grad. boost. trees	500	pos. & neg.
UCI Nomao	8	27,572	6,893	Grad. boost. trees	500	pos. & neg.
Real-world 1	16	183,755	45,940	Lattices	5	neg. only
Real-world 2	30	83,817	20,955	Lattices	500	neg. only

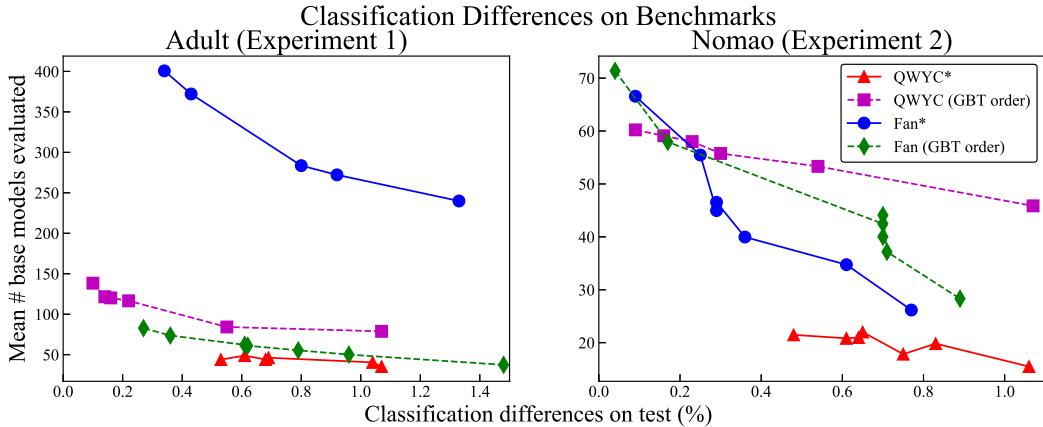


Figure 3: Classification differences vs. mean # base models evaluated for Adult and Nomao experiments.

D.2 Additional Discussion of Benchmark Experiments 1 and 2

Figure 1 illustrates the tradeoff between the mean number of base trees and the test accuracy for both the Adult and Nomao experiments. Notably, Figure 1 includes the baseline where we trained smaller gradient boosted tree ensembles (“GBT alone”). The comparison of QWYC* to GBT alone shows that one can achieve better accuracy by training a larger ensemble of 500 base models and dynamically pruning it down to 40 base models using QWYC* than by training an ensemble of 40 base models in the first place.

D.3 Independently-trained Real-World Experiments

Experiment 5: Real-World 1, Independently Trained: In this experiment, we use the same setup as Experiment 3, except the base models are independently trained instead of jointly trained.

Experiment 6: Real-World 2, Independently Trained: In this experiment, we use the same setup as Experiment 4, except the base models are independently trained instead of jointly trained.

For both real-world datasets, we see better speedups for independently trained ensembles than for jointly trained ensembles. This is likely because when independently-trained, each base model correlates more strongly with the full evaluation than when the ensemble is jointly-trained. This effect is most pronounced for real-world dataset 1, with an average 4x speed-up for the independently-trained ensemble (Table 4) compared to a 2.7x speedup for the jointly-trained ensemble (Table 2). The difference is much smaller for real-world dataset 2, but the mean number of base models evaluated is slightly lower for QWYC in Table 5.

For independently trained ensembles, the ordering mattered less, and a random ordering sometimes produced even better speed-ups than the other more “clever” fixed orderings. In Experiment 6, Figure 4, the random orderings performed significantly better than both Greedy MSE and Individual MSE orderings. Even in cases where the more “clever” Greedy MSE and Individual MSE orderings failed, QWYC’s joint optimization of ordering and thresholds in Algorithm 1 was able to replicate at least statistically similar performance to the best random ordering.

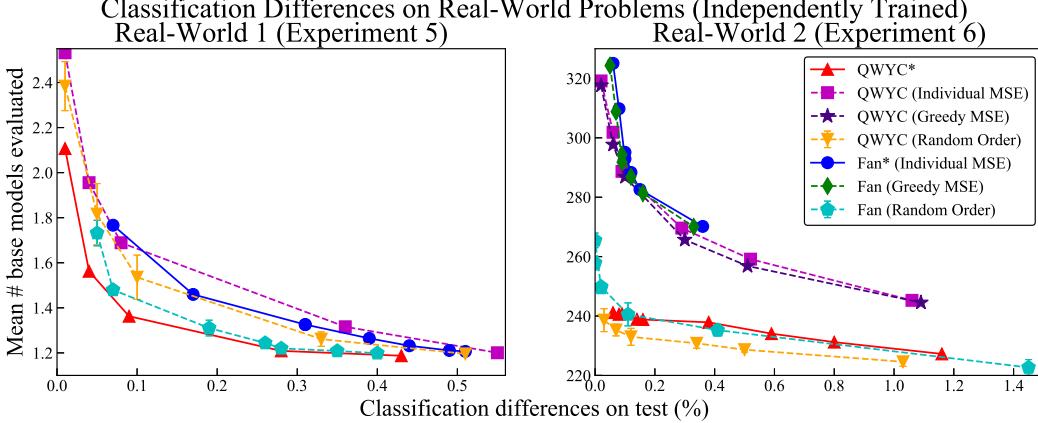


Figure 4: Classification differences vs. mean # base models evaluated for real-world experiments with independently trained ensembles.

Table 2: Experiment 3 - Comparison of Evaluation Times for Jointly Trained Ensemble of 5 Base Models.

Algorithm	Test % Diff	Test Mean # Base Models	Test Mean μs Eval Time	Test Mean Speed-up
Full ens.	0	5	$4.98 \pm 6\%$	1x
QWYC	0.44%	1.54	$1.82 \pm 7\%$	2.7x
Fan	0.51%	2.09	$2.49 \pm 8\%$	2.0x

Table 3: Experiment 4 - Comparison of Evaluation Times for Jointly Trained Ensemble of 500 Base Models

Algorithm	Test % Diff	Test Mean # Base Models	Test Mean μs Eval Time	Test Mean Speed-up
Full ens.	0	500	$322 \pm 4\%$	1x
QWYC	0.45%	237	$177 \pm 4\%$	1.8x
Fan	0.46%	309	$293 \pm 12\%$	1.1x

Table 4: Experiment 5 - Comparison of Evaluation Times for Independently Trained Ensemble of 5 Base Models

Algorithm	Test % Diff	Test Mean # Base Models	Test Mean μs Eval Time	Test Mean Speed-up
Full ens.	0	5	$4.91 \pm 7\%$	1x
QWYC	0.43%	1.18	$1.23 \pm 6\%$	4.0x
Fan	0.51%	1.20	$1.39 \pm 7\%$	3.5x

D.4 Distributions of # base models evaluated per test example

Figures 5 and 6 show the distribution across the test set for the number of base models evaluated per example. QWYC exhibits among the smoothest tapering behavior, where the number of examples evaluated with t base models decreases exponentially as t increases.

Table 5: Experiment 6 - Comparison of Evaluation Times for Independently Trained Ensemble of 500 Base Models

Algorithm	Test % Diff	Test Mean # Base Models	Test Mean μs Eval Time	Test Mean Speed-up
Full ens.	0	500	$269 \pm 4\%$	1x
QWYC	0.59%	234	$149 \pm 4\%$	1.8x
Fan	0.46%	268	$209 \pm 7\%$	1.3x

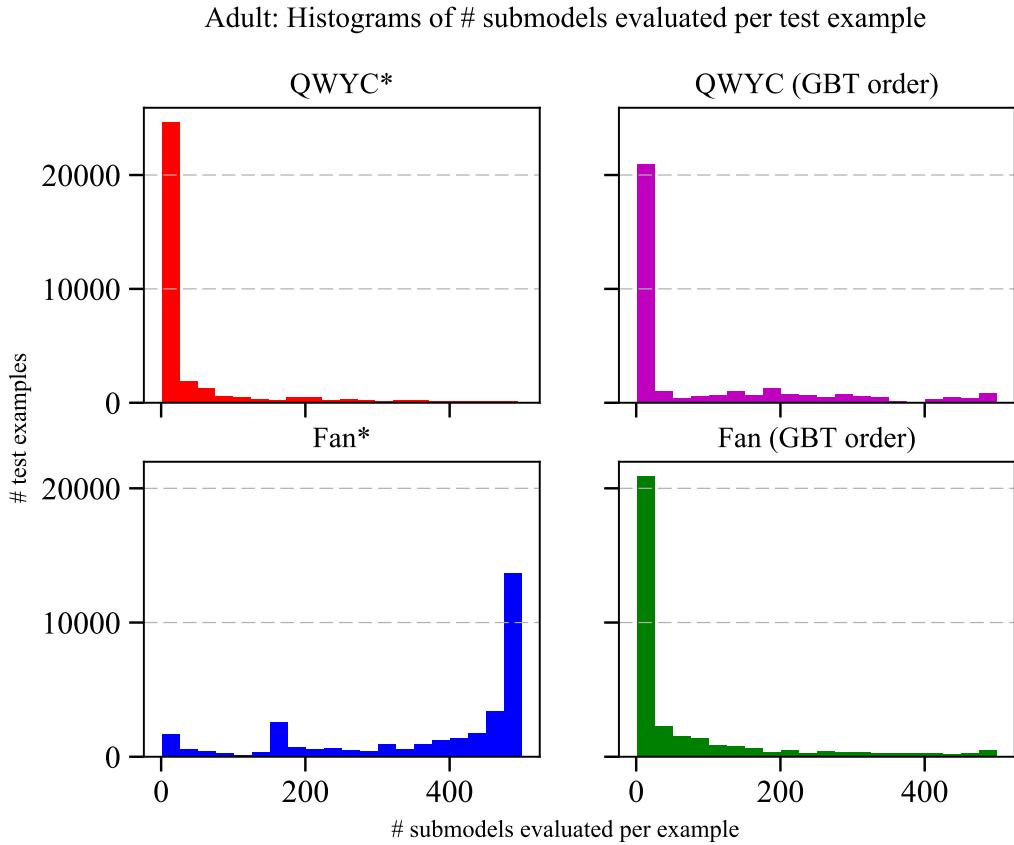


Figure 5: Histograms showing the distribution of the number of base models evaluated per example across the test dataset on Adult, for models that exhibit $\approx 0.5\%$ classification differences to the full ensemble on the test set.

Nomao: Histograms of # submodels evaluated per test example

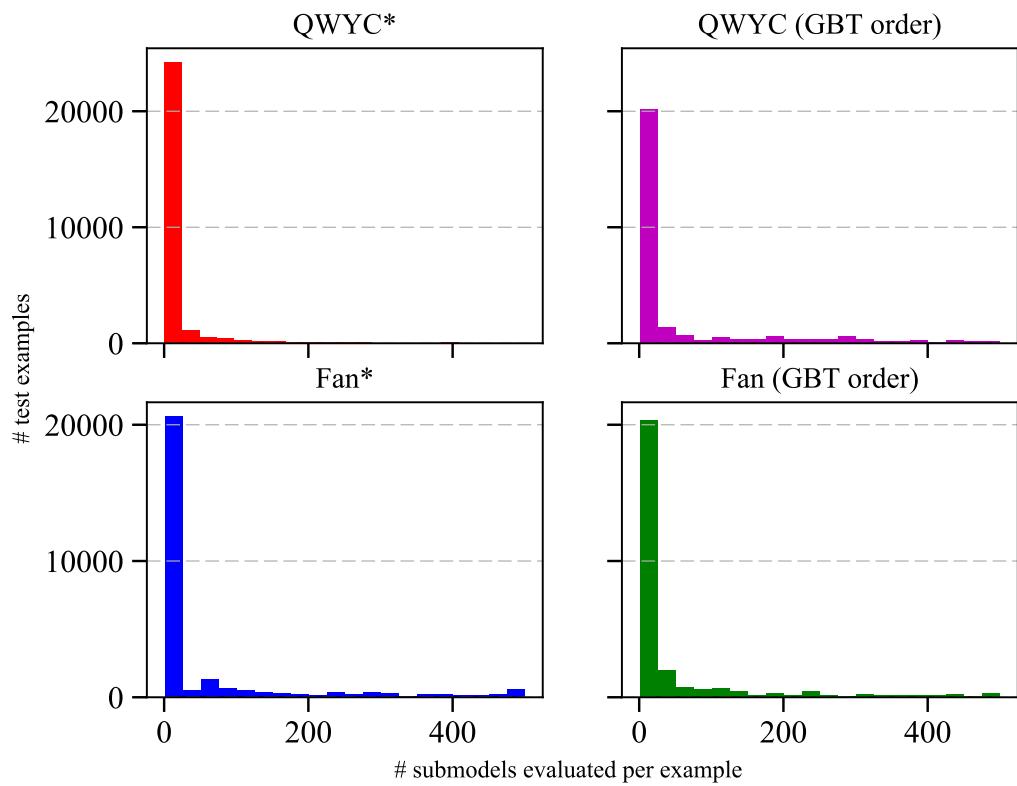
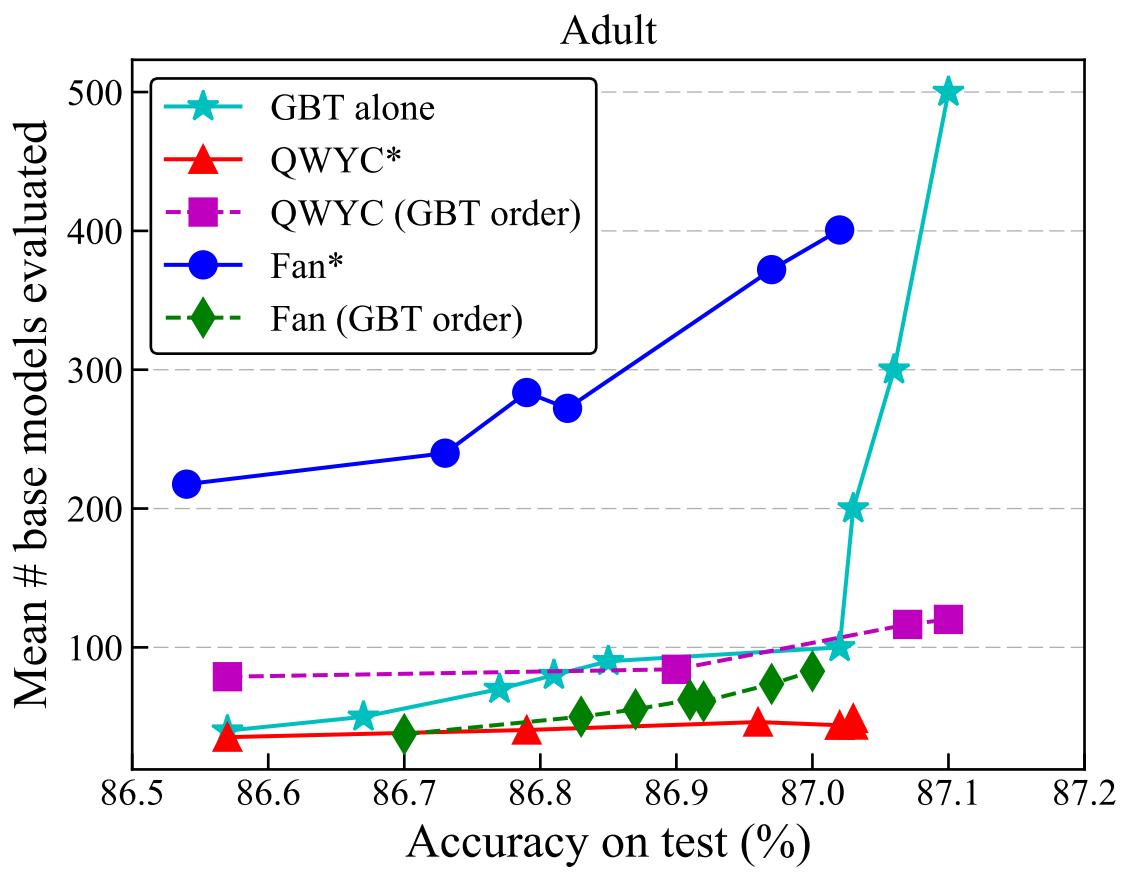


Figure 6: Histograms showing the distribution of the number of base models evaluated per example across the test dataset on Nomao, for models that exhibit $\approx 0.5\%$ classification differences to the full ensemble on the test set.



Nomao

