

LEVERAGING SIMPLE MODEL PREDICTIONS FOR ENHANCING ITS PERFORMANCE

Anonymous authors
Paper under double-blind review

ABSTRACT

There has been recent interest in improving performance of simple models for multiple reasons such as interpretability, robust learning from small data, deployment in memory constrained settings as well as environmental considerations. In this paper, we propose a novel method SRatio that can utilize information from high performing complex models (viz. deep neural networks, boosted trees, random forests) to reweight a training dataset for a potentially low performing simple model such as a decision tree or a shallow network enhancing its performance. Our method also leverages the per sample hardness estimate of the simple model which is not the case with the prior works which primarily consider the complex model’s confidences/predictions and is thus conceptually novel. Moreover, we generalize and formalize the concept of attaching probes to intermediate layers of a neural network, which was one of the main ideas in previous work (Dhurandhar et al., 2018b), to other commonly used classifiers and incorporate this into our method. The benefit of these contributions is witnessed in the experiments where on 6 UCI datasets and CIFAR-10 we outperform competitors in a majority (16 out of 27) of the cases and tie for best performance in the remaining cases. In fact, in a couple of cases, we even approach the complex model’s performance. We also conduct further experiments to validate assertions and intuitively understand why our method works. Theoretically, we motivate our approach by showing that the weighted loss minimized by simple models using our weighting upper bounds the loss of the complex model.

1 INTRODUCTION

Simple models such as decision trees or rule lists or shallow neural networks still find use in multiple settings where a) (global) interpretability is needed, b) small data sizes are available, or c) memory/computational constraints are prevalent (Dhurandhar et al., 2018b). In such settings compact or understandable models are often preferred over high performing complex models, where the combination of a human with an interpretable model can have better on-field performance than simply using the best performing black box model (Varshney et al., 2018). For example, a manufacturing engineer with an interpretable model may be able to obtain precise knowledge of how an out-of-spec product was produced and can potentially go back to fix the process as opposed to having little-to-no knowledge of how the decision was reached. Posthoc local explainability methods (Ribeiro et al., 2016; Bach et al., 2015; Dhurandhar et al., 2018a) can help delve into the local behavior of black box models, however, besides the explanations being only local, there is no guarantee that they are in fact true (Rudin, 2018). There is also a growing concern of the carbon footprint left behind in training complex deep models (Strubell et al., 2019), which for some popular architectures is more than that left behind by a car over its entire lifetime.

In this paper, we propose a method, SRatio, which reweights the training set to improve simple models given access to a highly accurate complex model such as a deep neural network, boosted trees, or some other predictive model. Given the applications we are interested in such as interpretability or deployment of models in resource limited settings, we assume the complexity of the simple models to be predetermined or fixed (viz. decision tree of height ≤ 5), where we cannot grow arbitrary size ensembles such as in boosting or bagging (Freund & Schapire, 1997). Our method applies potentially to any complex-simple model combination which is not the case for some state-of-the-art methods in

this space such as Knowledge Distillation (Geoffrey Hinton, 2015) or Profweight (Dhurandhar et al., 2018b), where the complex model is assumed to be a deep neural network. In addition, we generalize and formalize the concept of probes presented in (Dhurandhar et al., 2018b) and provide examples of what they would correspond to for classifiers other than neural networks, which our method is able to leverage. Our method also uses the a priori low performing simple models confidences to enhance its performance which we believe is conceptually novel compared to the existing methods which seem to *only* leverage the complex model (viz. its predictions/confidences). The benefit of this is seen in experiments where we outperform other competitors in a majority of the cases and are tied with one or more methods for best performance in the remaining cases. In fact, in a couple of cases we even approach the complex model’s performance, i.e. a single tree is made to be as accurate as 100 boosted trees. Moreover, we motivate our approach by contrasting it with covariate shift and show that our weighting scheme where we now minimize the weighted loss of the simple model is equivalent to minimizing an upper bound on the loss of the complex model for commonly used loss functions such as cross-entropy loss, least squares loss, and hinge loss.

2 RELATED WORK

Knowledge Distillation (Geoffrey Hinton, 2015; Tan et al., 2017; Lopez-Paz et al., 2016) is one of the most popular approaches for building "simpler" neural networks. It typically involves minimizing the cross-entropy loss of a simpler network based on calibrated confidences (Guo et al., 2017) of a more complex network. The simpler networks are usually not that simple in that they are typically of the same (or similar) depth but thinned down (Romero et al., 2015). This is generally insufficient to meet tight resource constraints (Reagen et al., 2016). Moreover, the thinning down was shown for convolutional neural networks but it is unclear how one would do the same for modern architectures such as ResNets. The weighting of training inputs approach on the other hand can be more easily applied to different architectures. It also has another advantage in that it can be readily applied to models optimizing losses other than cross-entropy (viz. hinge loss, squared loss) with some interpretation of which inputs are more (or less) important. Some other strategies to improve simple models (Buciluă et al., 2006; Ba & Caurana, 2013; Bastani et al., 2017) are also conceptually similar to Distillation, where the actual outputs are replaced by predictions from the complex model.

The most relevant work to our current endeavor is ProfWeight (Dhurandhar et al., 2018b), where they too weight the training inputs. Their method however, requires the complex model to be a neural network and thus does not apply to settings where we have a different complex model. Moreover, their method like Distillation takes into account only the complex models assessment of the difficulty of an example.

Curriculum learning (CL) (Bengio et al., 2009) and boosting (Freund & Schapire, 1997) are two other approaches which rely on weighting samples, however, their motivation and setup are significantly different. In both CL and boosting the complexity of the improved learner can increase as they do not have to respect constraints such as interpretability (Dhurandhar et al., 2017; Montavon et al., 2017) or limited memory/power (Reagen et al., 2016; Chen et al., 2016). In CL typically, there is no automatic gradation of example difficulty during training. While in boosting the examples are graded with respect to a previous weak learner and not an independent accurate complex model. Also, as we later show, our method does not necessarily up-weight hard examples but rather uses a measure that takes into account hardness as assessed by both the complex and simple models.

3 METHODOLOGY

In this section, we first provide theoretical and intuitive justification for our approach. This is followed by description of our method which utilizes the notion of graded classifiers that we formally define and also provide practical examples for.

3.1 THEORETICAL MOTIVATION

Our approach in section 3.3 can be motivated by contrasting it with the covariate shift (Agarwal et al., 2011) setting. If $X \times Y$ is the input-output space and $p(x, y)$ and $q(x, y)$ are the source and target distributions in the covariate shift setting, then it is assumed that $p(y|x) = q(y|x)$ but

$p(x) \neq q(x)$. One of the standard solutions for such settings is importance sampling where the source data is sampled proportional to $\frac{q(x)}{p(x)}$ in order to mimic as closely as possible the target distribution. In our case, the dataset is the same but the classifiers (i.e. complex and simple) are different. We can think of this as a setting where $p(x) = q(x)$ as both the models learn from the same data, however, $p(y|x) \neq q(y|x)$ where $p(y|x)$ and $q(y|x)$ correspond to the outputs of complex and simple classifiers, respectively. Given that we want the simple model to approach the complex models performance a natural analog to the importance weights used in covariate shift is to weight samples by $\frac{p(y|x)}{q(y|x)}$ in our setting which is the essence of our method as described below in section 3.3.

We now show that for different commonly used loss functions such a weighting applied to the simple model’s loss upper bounds the loss of the complex model (proof in appendix) subject to an intuitive assumption on the weights which is justified in the following section.

Lemma 3.1. *If λ denotes cross-entropy loss, squared loss or hinge loss with $w = \frac{p(y|x)}{q(y|x)} \geq 1$, then $\lambda(p(y|x)) \leq w\lambda(q(y|x))$.*

Now, let us formally show that for cross-entropy loss even with the weaker assumption that the (expected) loss of the complex model is no greater than the simple model reweighing and training the simple model is a valid and sound procedure by demonstrating that it is upper bound on the loss we want to ideally optimize.

Lemma 3.2. *Let $p_\theta(y|x)$ be the softmax scores on a specific model θ from simple model space Θ . Let θ^* be the optimal model that minimizes $\mathbb{E}[-\log p_\theta(y|x)]$ on the training distribution from Θ . Let $p_c(y|x)$ be a pretrained complex classifier whose loss is smaller than θ^* on the training distribution. Then we have:*

$$\begin{aligned} \mathbb{E}[-\log p_\theta(y|x)] &\leq \mathbb{E} \left[\max \left(1, \frac{p_c(y|x)}{p_{\theta^*}(y|x)} \right) \log \left(\frac{1}{p_\theta(y|x)} \right) \right] + \mathbb{E}[\log p_{\theta^*}(y|x)] \\ &\quad + \mathbb{E}[-\log p_c(y|x)] \end{aligned} \quad (1)$$

Proof.

$$\begin{aligned} \mathbb{E}[-\log(p_\theta(y|x))] &= \mathbb{E} \left[\log \left(\frac{1}{p_\theta(y|x)} * \frac{p_c(y|x)}{p_{\theta^*}(y|x)} \right) \right] - \mathbb{E}[\log \left(\frac{p_c(y|x)}{p_{\theta^*}(y|x)} \right)] \\ &\leq \mathbb{E} \left[\log \left(\frac{1}{p_\theta(y|x)} * \max \left(1, \frac{p_c(y|x)}{p_{\theta^*}(y|x)} \right) \right) \right] - \mathbb{E}[\log \left(\frac{p_c(y|x)}{p_{\theta^*}(y|x)} \right)] \\ &\stackrel{a}{\leq} \mathbb{E} \left[\max \left(1, \frac{p_c(y|x)}{p_{\theta^*}(y|x)} \right) \log \left(\frac{1}{p_\theta(y|x)} \right) \right] + \mathbb{E}[\log p_{\theta^*}(y|x)] \\ &\quad + \mathbb{E}[-\log p_c(y|x)] \end{aligned} \quad (2)$$

(a) It uses the following inequality: $\log(wx) \leq w \log(x)$, $w \geq 1$, $x > 1$ as \log is a positive value monotonically increasing function in $[1, \infty]$. \square

Remark: We observe that re-weighting every sample by $\max(1, \frac{p_c(y|x)}{p_{\theta^*}(y|x)})$ and re-optimizing using the simple model training algorithm is a sound way to optimize the cross entropy loss of the simple model on the training data set. The reason we believe that optimizing the upper bound could be better is because many simple models such as decision trees are trained using a simple greedy approach. Therefore, reweighting samples based on an accurate complex model could induce the appropriate bias leading to better solutions. Moreover, in equation 2, the second inequality is the main place where there is slack between the upper bound and the quantity we are interested in bounding. This inequality is tightest if $w = \frac{p_c(y|x)}{p_{\theta^*}(y|x)}$ is not much bigger than 1 on average. Optimizing the simple model using its training procedure on the weighted dataset would be one of the ways to ensure this ratio is close to 1.

3.2 INTUITIVE JUSTIFICATION

Intuitively, assuming $w \geq 1$ implies that the complex model finds an input easier (i.e. higher score or confidence) to classify in the correct class than does the simple model. Although in practice this

Algorithm 1 Our proposed method SRatio.

Input: n (graded) classifiers ζ_1, \dots, ζ_n , learning algorithm for simple model \mathcal{L}_S , dataset D_S of cardinality N , performance gap parameter γ and maximum allowed ratio parameter β .

- 1) Train simple model on D_S , $\mathcal{S} \leftarrow \mathcal{L}_S(D_S, \vec{1}_N)$ and compute its (average) prediction error ϵ_S . {Obtain initial simple model where each input is given a unit weight.}
 - 2) Compute (average) prediction errors $\epsilon_1, \dots, \epsilon_n$ for the n graded classifiers and store the ones that are at least γ more accurate than the simple model i.e. $I \leftarrow \{i \in \{1, \dots, n\} \mid \epsilon_S - \epsilon_i \geq \gamma\}$
 - 3) Compute weights for all inputs x as follows: $w(x) = \frac{\sum_{i \in I} \zeta_i(x)}{m\mathcal{S}(x)}$, where m is the cardinality of set I and $\mathcal{S}(x)$ is the prediction probability/score for the true class of the simple model.
 - 4) Set $w(x) \leftarrow 0$, if $w(x) > \beta$. {Ignore extremely hard examples for the simple model.}
 - 5) Retrain the simple model on the dataset D_S with the corresponding learned weights \mathbf{w} , $\mathcal{S}_w \leftarrow \mathcal{L}_S(D_S, \mathbf{w})$
 - 6) **Return** \mathcal{S}_w
-

may not always be the case, it is not unreasonable to believe that this would occur for most inputs, especially if the complex model is highly accurate.

The motivation for our approach conceptually does not contradict (Dhurandhar et al., 2018b), where hard samples for a complex model are weighted low. These would still be potentially weighted low as the numerator would be small. However, the main difference would occur in the weighting of the easy examples for the complex model, which rather than being uniformly weighted high would now be weighted based on the assessment of the simple model. This, we believe, is important information as stressing inputs that are already extremely easy for the simple model to classify will possibly not lead to the best generalization. It is probably more important to stress on inputs that are somewhat hard for the simple model but easier for the complex model, as that is likely to be the critical point of information transfer. Thus, even though easier inputs for the complex model are likely to get higher weights ranking these based on the simple models assessment is important and not captured in the previous approaches. Hence, although our idea may appear to be simple, we believe it is a significant jump conceptually in that it also takes into account the simple model’s behavior to improve itself.

Our method described in the next section is a generalization of this idea and the motivation presented in the previous section. If the confidences of the complex model are representative of difficulty then we could leverage them alone, however, many times as seen in previous work (Dhurandhar et al., 2018b), they may not be and hence using confidences of lower layers or simpler forms of the complex classifier can be very helpful.

3.3 METHOD

We now present our approach SRatio in algorithm 1, which uses the ideas presented in the previous sections and generalizes the method in (Dhurandhar et al., 2018b) to be applicable to complex classifiers other than neural networks.

In previous works (Akshayvarun Subramanya, 2017; Dhurandhar et al., 2018b), it was seen that sometimes highly accurate models such as deep neural networks may not be good density estimators and hence may not provide an accurate quantification of the relative difficulty of an input. To obtain a better quantification, the idea of attaching probes (viz. linear classifiers) to intermediate layers of a deep neural network and then averaging the confidences was proposed. This, as seen in the previous work, led to significantly better results over the state-of-the-art. Similarly, we generalize our method where rather than taking just the output confidences of the complex model as the numerator, we take an average of the confidences over a gradation of outputs produced by taking appropriate simplifications of the complex model. We formalize this notion of graded outputs as follows:

Definition (δ -graded) Let $X \times Y$ denote the input-output space and $p(x, y)$ the joint distribution over this space. Let $\zeta_1, \zeta_2, \dots, \zeta_n$ denote classifiers that output the prediction probabilities for a given input $x \in X$ for the most probable (or true) class $y \in Y$ determined by $p(y|x)$. We then say that classifiers $\zeta_1, \zeta_2, \dots, \zeta_n$ are δ -graded for some $\delta \in (0, 1]$ and a (measurable) set $Z \subseteq X$ if $\forall x \in Z$, $\zeta_1(x) \leq \zeta_2(x) \leq \dots \leq \zeta_n(x)$, where $\int_{x \in Z} p(x) \geq \delta$.

Loosely speaking, the above definition says that a sequence of classifiers is δ -graded if a classifier in the sequence is at least as accurate as the ones preceding it for at least δ measure of the inputs. Thus, a sequence would be 1-graded if the above inequalities were true for the entire input space (i.e. $Z = X$). Below are some examples of how one could produce δ -graded classifiers for different models in practice, for possibly large enough δ s.

- **Deep Neural Networks:** The notion of attaching probes, which are essentially linear classifiers (viz. $\sigma(Wx + b)$) trained on intermediate layers of a deep neural network (Dhurandhar et al., 2018b; Alain & Bengio, 2016) could be seen as a way of creating δ -graded classifiers, where lower layer probes are likely to be less accurate than those above them for most of the samples. Thus the idea of probes used in previous works as simplifications of the complex model are captured by our definition.
- **Boosted Trees:** One natural way here could be to just consider the ordering produced by boosting algorithms that grow the tree ensemble and use all the trees up to a certain point. For example, if we have an ensemble of 10 trees, then ζ_1 could be the first tree, ζ_2 could be the first two trees and so on where ζ_{10} is the entire ensemble.
- **Random Forests:** Here one could order trees based on performance and then do a similar grouping as above where ζ_1 could be the least accurate tree, then ζ_2 could be the ensemble of ζ_1 and the second most inaccurate tree and so on. Of course, for this and boosted trees one could take bigger steps and add more trees to produce the next ζ so that there is a measurable jump in performance from one graded classifier to the next.
- **Other Models:** For non-ensemble models such as generalized linear models one too could form graded classifiers by taking say different order Taylor approximations of the functions or by setting the least important coefficients successively to zero by doing function decompositions based on binary, ternary and higher order interactions (Molnar et al., 2019), or using feature selection and starting with a model containing the most important feature(s).

Given this, we see in algorithm 1 that we take as input graded classifiers and the learning algorithm for the simple model. Trivially, the graded classifiers can just be the entire complex classifier where we only consider its output confidences. We now take a ratio of the average confidence of the graded classifiers that are at least more accurate than the simple model by $\gamma > 0$ and the simple model's confidence. If this ratio is too large (i.e. $> \beta$) we set the weight to zero and otherwise the ratio is the weight for that input. Note that setting large weights to zero reduces the variance of the simple model because it prevents dependence on a select few examples. Moreover, large weights mostly indicate that the input is extremely hard for the simple model to classify correctly and so expending effort on it and ignoring other examples will most likely be detrimental to performance. Best values for both parameters can be found empirically using standard validation procedures.

4 EXPERIMENTS

In this section, we empirically validate our approach as compared with other state-of-the-art methods used to improve simple models. We experiment on 6 real datasets from UCI (Dheeru & Karra Taniskidou, 2017): Ionosphere, Ovarian Cancer (OC), Heart Disease (HD), Waveform, Human Activity Recognition (HAR), and Musk. Data characteristics are given in the appendix.

4.1 UCI DATASETS SETUP

We experiment with two complex models, namely, boosted trees and random forests, each of size 100. For each of the complex models we see how the different methods perform in enhancing two simple models: a single CART decision tree and a linear SVM classifier. Since ProfWeight is not directly applicable in this setting, we compare with its special case ConfWeight which weighs examples based on the confidence score of the complex model. We also compare with an equivalent model to Distillation since it is mainly designed for cross-entropy loss, where the simple model is trained on the complex models predictions. Datasets are randomly split into 70% train and 30% test. Results for all methods are averaged over 10 random splits and reported in Table 1 with 95% confidence intervals.

Table 1: Below we see the averaged % errors with 95% confidence intervals for the different methods on six real datasets. Boosted Trees and Random Forest (100 trees) are the complex models (CM), while a single decision tree and linear SVM are the simple models (SM). Best simple model results are indicated in bold. * indicates the simple model has approached the complex models performance.

Dataset	Complex Model	CM Error	Simple Model	SM Error	Distillation Error (SM)	ConfWeight Error (SM)	SRatio Error (SM)
Ionosphere	Boosted Trees	8.10 ±0.4	Tree	10.95 ±0.4	10.95 ±0.4	11.42 ±0.8	8.57* ±0.5
			SVM	12.38 ±0.6	11.90 ±0.6	11.90 ±0.6	10.47 ±0.5
	Random Forest	6.19 ±0.4	Tree	10.95 ±0.4	10.95 ±0.4	11.42 ±0.4	10.42 ±0.1
			SVM	12.38 ±0.6	12.38 ±0.6	12.38 ±0.6	11.42 ±0.3
Ovarian Cancer	Boosted Trees	4.68 ±0.4	Tree	15.62 ±0.8	15.62 ±0.8	15.62 ±1.0	15.62 ±0.5
			SVM	1.56 ±0.4	1.56 ±0.4	1.56 ±0.4	1.56 ±0.4
	Random Forest	6.25 ±0.8	Tree	15.62 ±0.8	15.62 ±0.8	14.06 ±0.1	14.04 ±0.1
			SVM	1.56 ±0.4	1.56 ±0.4	1.56 ±0.4	1.56 ±0.4
Heart Disease	Boosted Trees	15.55 ±0.6	Tree	23.88 ±0.7	22.77 ±0.1	23.33 ±0.3	22.77 ±0.2
			SVM	17.22 ±0.2	16.67 ±0.3	17.22 ±0.2	16.77 ±0.2
	Random Forest	15.88 ±0.6	Tree	23.88 ±0.7	23.88 ±0.7	25.55 ±0.5	22.77 ±0.3
			SVM	17.22 ±0.2	17.22 ±0.2	16.67 ±0.3	16.67 ±0.2
Waveform	Boosted Trees	12.96 ±0.1	Tree	25.43 ±0.2	25.06 ±0.1	25.10 ±0.1	25.06 ±0.1
			SVM	14.70 ±0.2	15.33 ±0.0	14.70 ±0.2	13.72 ±0.2
	Random Forest	10.90 ±0.1	Tree	25.43 ±0.2	25.43 ±0.2	25.43 ±0.2	25.06 ±0.1
			SVM	14.70 ±0.2	14.33 ±0.0	14.30 ±0.2	12.72 ±0.5
Human Activity Recognition	Boosted Trees	6.32 ±0.0	Tree	7.93 ±0.2	7.93 ±0.1	7.86 ±0.2	7.15 ±0.1
			SVM	14.56 ±0.1	15.85 ±0.1	13.92 ±0.1	13.92 ±0.2
	Random Forest	2.34 ±0.0	Tree	7.93 ±0.2	7.23 ±0.1	7.21 ±0.1	6.67 ±0.0
			SVM	14.56 ±0.1	13.92 ±0.1	14.24 ±0.1	13.92 ±0.1
Musk	Boosted Trees	4.06 ±0.1	Tree	4.49 ±0.1	6.11 ±0.1	4.45 ±0.1	4.06* ±0.1
			SVM	6.11 ±0.1	6.29 ±0.1	6.41 ±0.1	5.48 ±0.1
	Random Forest	2.45 ±0.1	Tree	4.49 ±0.1	4.49 ±0.1	4.47 ±0.1	3.89 ±0.1
			SVM	6.11 ±0.1	6.16 ±0.1	5.96 ±0.1	5.53 ±0.1

For our method, graded classifiers based on the complex models are formed as described before in steps of 10 trees. We have 10 graded classifiers ($10 \times 10 = 100$ trees) for both boosted trees and random forests. The trees in the random forest are ordered based on increasing performance. Optimal values for γ and β are found using 10-fold cross-validation.

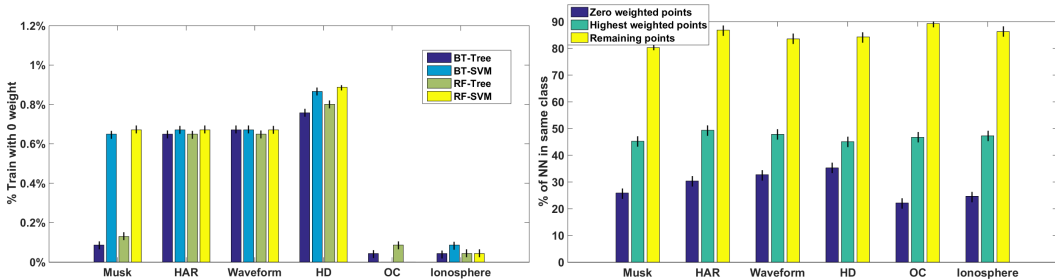


Figure 1: Above (left) we see the % of training set points assigned weight 0 by SRatio at optimal β values for each complex (BT, RF) and simple model (Tree, SVM) combination on the 6 UCI datasets. We see that $< 1\%$ of the training set has weights 0 in all cases. For Ovarian Cancer (OC) SVM was better than the complex models and hence no points had weight 0. Above (right) we analyze why intuitively our reweighting seems to work. The results are averaged over all complex-simple model combinations. Given 10 nearest neighbors (NN) of a data point, let ν_s and ν_d denote the number of those NNs that belong to its class (i.e. same class), and most frequent different class respectively. Then the Y-axis depicts $\frac{\nu_s}{\nu_s + \nu_d} \times 100$. This metric gives a feel for how difficult it is likely to be to correctly classify a point. We thus see that most of the 10 NNs for the 0 weight points lie in a different class, while for the highest weighted points (i.e. top 5 percentile) the % of NNs in the same class are almost 50%. This showcases why the 0 weight points are so difficult for the simple models to classify, while the highest weighted points seem to outline an important decision boundary (since same class NNs are close to 50%) and are relatively easier although one has to focus on them (since same class NNs still $< 50\%$) to classify them correctly. Qualitatively similar results were seen for 5-NN and 15-NN. Both plots represent averaged values over 10 random train/test splits with 95% confidence intervals.

4.2 CIFAR-10 SETUP

The setup we follow here is very similar to previous works (Dhurandhar et al., 2018b). The complex model is an 18 unit ResNet with 15 residual (Res) blocks/units. We consider a simple model that consists of 3 Res units, 5 Res units and 7 Res units. Each unit consists of two 3×3 convolutional layers with either 64, 128, or 256 filters (the exact architecture is given in the appendix). A 3×3 convolutional layer with 16 filters serves an input to the first ResNet block, while an average pooling layer followed by a fully connected layer with 10 logits takes as input the output of the final ResNet block for each of the models.¹

We form 18 graded classifiers by training probes which are linear classifiers with softmax activations attached to flattened intermediate representations corresponding to the 18 units of ResNet (15 Res units + 3 others). As done in prior studies, we split the 50000 training samples from the CIFAR-10 dataset into two training sets of 30000 and 20000 samples, which are used to train the complex and simple models, respectively. 500 samples from the CIFAR-10 test set are used for validation and hyperparameter tuning (details in appendix). The remaining 9500 are used to report accuracies of all the models. Distillation (Geoffrey Hinton, 2015) employs cross-entropy loss with soft targets to train the simple model, which are the softmax outputs of the complex model’s last layer rescaled by temperature $t = 0.5$ which was selected based on cross-validation. For ProfWeight, we report results for the area under the curve (AUC) version as it had the best performance in a majority of the cases in the prior study. Details of β and γ values that we experimented with to obtain the results in Table 2 are in the appendix.

4.3 OBSERVATIONS

In the experiments on the 6 UCI datasets depicted in Table 1, we observe that we are consistently the best performer, either tying or superseding other competitors. Given the 24 experiments based on dataset, complex model, and simple model combinations ($6 \times 2 \times 2 = 24$), we are the outright best performer in 14 of those cases, while being tied with one or more other methods for best performance in the remaining 10 cases. In fact, in 2 cases where we are outright best performers,

¹Tensorflow 1.5.0 was used for CIFAR-10 experiments

Table 2: Below we observe the averaged accuracies (%) of simple models SM-3 (3 Res units), SM-5 (5 Res units) and SM-7 (7 Res units) trained with various weighting methods and distillation. The complex model achieved 84.5% accuracy. Statistically significant best results are indicated in bold.

	SM-3	SM-5	SM-7
Standard	73.15 (± 0.7)	75.78 (± 0.5)	78.76 (± 0.35)
ConfWeight	76.27 (± 0.48)	78.54 (± 0.36)	81.46 (± 0.50)
Distillation	65.84 (± 0.60)	70.09 (± 0.19)	73.4 (± 0.64)
ProfWeight	76.56 (± 0.51)	79.25 (± 0.36)	81.34 (± 0.49)
SRatio	77.23 (± 0.14)	80.14 (± 0.22)	81.89 (± 0.28)

dataset=Ionosphere, complex model =boosted trees, simple model = Tree and dataset=Musk, complex model =boosted trees, simple model = Tree, our method enhances the simple model’s performance to match (statistically) that of the complex model which we believe to be a significant. In fact, on the Musk dataset, we observe that the simple tree model enhanced using our method, where the complex model is a random forest, supersedes the performance of the other complex model. On the Ovarian Cancer dataset, linear SVM actually seems to perform best, even better than the complex models. A reason for this may be that the dataset is high dimensional with few examples. Due to this, it also seems difficult for any of the methods to boost the simple model’s performance.

We now offer an intuition as to why our weighting works. First, we see in figure 1(left) that our assertion of only a very small fraction of the training set being assigned 0 weights based on parameter β , which upper bounds the weights, is true ($< 1\%$ is assigned weight 0). In figure 1(right), we see the intuitive justification for the learned weights. The 0 weighted points have very few nearest neighbors that are in the same class and so likely are almost impossible for a simple model to classify correctly. The highest weighted points have nearest neighbors from the same class that are close to the most frequent (different) class and hence possibly highlight an important decision boundary. With some effort a simple model should be able to classify them correctly and so focusing on them is important. The remaining points (on average) seem to be relatively easy for both complex and simple models.

On the CIFAR-10 dataset, we see that our method outperforms other state-of-the-art methods where simple model has 3 Res units and 5 Res units. For 7 Res units we tie with ProfWeight and ConfWeight. Given the motivation of resource limited settings where memory constraints can be stringent (Reagen et al., 2016; Chen et al., 2016), SM-3 and SM-5 are anyway the more reasonable options. In general, we see from these experiments that the simple models predictions can be highly informative in improving its own performance.

5 DISCUSSION

Our approach and results outline an interesting strategy, where even in cases that one might want a simple model, it might be beneficial to build an accurate complex model first and use it to enhance the desired simple model. Such is exactly the situation for the manufacturing engineer described in the introduction that has experience with simple interpretable models that provide him with knowledge that a complex model with better performance cannot offer.

Although our method may appear to be simplistic, we believe it to be a conceptual jump in that it takes into account the difficulty of a sample not just based on the complex model, but also the simple model which a priori is not obvious and hence possibly ignored by previous methods that may or may not be weighting-based. Moreover, we have empirically shown that our method either outperforms or matches the best solutions across a wide array of datasets for different complex model (viz. boosted trees, random forests and ResNets) and simple model (viz. single decision trees, linear SVM and small ResNets) combinations. In fact, in a couple of cases, a single tree approached the performance of a 100 boosted trees using our method. In addition, we also formalized and generalized the idea behind probes presented in previous work (Dhurandhar et al., 2018b), which were specific for deep neural networks, to other classifiers and gave examples of practical instantiations. In the future, we would like to uncover more such methods and study their theoretical underpinnings.

REFERENCES

- D. Agarwal, L. Li, and A. J. Smola. Linear-Time Estimators for Propensity Scores. In *14th Intl. Conference on Artificial Intelligence and Statistics (AISTATS)*, pp. 93–100, 2011.
- R. Venkatesh Babu Akshayvarun Subramanya, Suraj Srinivas. Confidence estimation in deep neural networks via density modelling. *arXiv preprint arXiv:1707.07013*, 2017.
- Guillaume Alain and Yoshua Bengio. Understanding intermediate layers using linear classifier probes. *arXiv preprint arXiv:1610.01644*, 2016.
- Lei Jimmy Ba and Rich Caurana. Do deep nets really need to be deep? *CoRR*, abs/1312.6184, 2013. URL <http://arxiv.org/abs/1312.6184>.
- Sebastian Bach, Alexander Binder, Grégoire Montavon, Frederick Klauschen, Klaus-Robert Müller, and Wojciech Samek. On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation. *PLoS one*, 10(7):e0130140, 2015.
- Osbert Bastani, Carolyn Kim, and Hamsa Bastani. Interpreting blackbox models via model extraction. *arXiv preprint arXiv:1705.08504*, 2017.
- Yoshua Bengio, Jérôme Louradour, Ronan Collobert, and Jason Weston. Curriculum learning. In *Proceedings of the 26th Annual International Conference on Machine Learning*, 2009.
- Cristian Buciluă, Rich Caruana, and Alexandru Niculescu-Mizil. Model compression. In *Proceedings of the 12th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 2006.
- Yu-Hsin Chen, Joel Emer, and Vivienne Sze. Eyeriss: A spatial architecture for energy-efficient dataflow for convolutional neural networks. In *2016 ACM/IEEE 43rd Annual International Symposium on Computer Architecture*, 2016.
- Dua Dheeru and Efi Karra Taniskidou. UCI machine learning repository, 2017. URL <http://archive.ics.uci.edu/ml>.
- Amit Dhurandhar, Vijay Iyengar, Ronny Luss, and Karthikeyan Shanmugam. Tip: Typifying the interpretability of procedures. *arXiv preprint arXiv:1706.02952*, 2017.
- Amit Dhurandhar, Pin-Yu Chen, Ronny Luss, Chun-Chen Tu, Paishun Ting, Karthikeyan Shanmugam, and Payel Das. Explanations based on the missing: Towards contrastive explanations with pertinent negatives. In *Advances in Neural Information Processing Systems 31*. 2018a.
- Amit Dhurandhar, Karthikeyan Shanmugam, Ronny Luss, and Peder Olsen. Improving simple models with confidence profiles. *Advances of Neural Inf. Processing Systems (NeurIPS)*, 2018b.
- Yoav Freund and Robert E. Schapire. Decision-theoretic generalization of on-line learning and an application to boosting. *Journal of Computer and System Sciences*, 55(1):119–139, 1997.
- Jeff Dean Geoffrey Hinton, Oriol Vinyals. Distilling the knowledge in a neural network. In <https://arxiv.org/abs/1503.02531>, 2015.
- Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Weinberger. On calibration of modern neural networks. *Intl. Conference on Machine Learning (ICML)*, 2017.
- David Lopez-Paz, Leon Bottou, Bernhard Schölkopf, and Vladimir Vapnik. Unifying distillation and privileged information. In *International Conference on Learning Representations (ICLR 2016)*, 2016. URL <http://leon.bottou.org/papers/lopez-paz-2016>.
- Christoph Molnar, Giuseppe Casalicchio, and Bernd Bischl. Quantifying interpretability of arbitrary machine learning models through functional decomposition. *CoRR*, 2019. URL <https://arxiv.org/abs/1904.03867>.
- Grégoire Montavon, Wojciech Samek, and Klaus-Robert Müller. Methods for interpreting and understanding deep neural networks. *Digital Signal Processing*, 2017.

Brandon Reagen, Paul Whatmough, Robert Adolf, Saketh Rama, Hyunkwang Lee, Sae Kyu Lee, Jose Miguel, Hernandez-Lobato, Gu-Yeon Wei, and David Brooks. Minerva: Enabling low-power, highly-accurate deep neural network accelerators. *IEEE Explore*, 2016.

Marco Ribeiro, Sameer Singh, and Carlos Guestrin. "why should i trust you?" explaining the predictions of any classifier. In *ACM SIGKDD Intl. Conference on Knowledge Discovery and Data Mining*, 2016.

Adriana Romero, Nicolas Ballas, Samira Ebrahimi Kahou, Antoine Chassang, Carlo Gatta, and Yoshua Bengio. Fitnets: Hints for thin deep nets. *arXiv preprint arXiv:1412.6550*, 2015.

Cynthia Rudin. Please stop explaining black box models for high stakes decisions. *NIPS Workshop on Critiquing and Correcting Trends in Machine Learning*, 2018.

Emma Strubell, Ananya Ganesh, and Andrew McCallum. Energy and policy considerations for deep learning in nlp. *CoRR*, 2019. URL <https://arxiv.org/abs/1906.02243>.

Sarah Tan, Rich Caruana, Giles Hooker, and Yin Lou. Auditing black-box models using transparent model distillation with side information. *CoRR*, 2017. URL <https://arxiv.org/abs/1710.06169>.

Kush R. Varshney, Prashant Khanduri, Pranay Sharma, Shan Zhang, and Pramod K. Varshney. Why interpretability in machine learning? an answer using distributed detection and data fusion theory. *ICML Workshop on Human Interpretability in Machine Learning (WHI)*, 2018.

A APPENDIX

Proof of Lemma 3.1

Proof. For cross-entropy loss, assume $q(y|x), p(y|x) \in [0, 1]$. Then

$$\begin{aligned} q(y|x)w &\geq q(y|x)^w \\ \log(q(y|x)w) &\geq w\log(q(y|x)) \\ -\log(q(y|x)w) &\leq -w\log(q(y|x)) \end{aligned}$$

For hinge loss, if y is the true label for an input, then

$$\begin{aligned} \max(0, 1 - yq(y|x)w) &\leq \max(0, w - yq(y|x)w) \\ &= \max(0, w(1 - yq(y|x))) \\ &= w \max(0, 1 - yq(y|x)) \end{aligned}$$

For squared loss if $y \in \{-1, 1\}$ is again the true label and hence $q(y|x), p(y|x) \in [-1, 1]$ are corresponding scoring functions for the simple and complex model, then

$$\begin{aligned} y^2 &\geq p(y|x)q(y|x) \\ \left(\frac{y}{q(y|x)}\right)^2 &\geq w \\ y^2 - wq(y|x)^2 &\geq 0 \\ (w-1)(y^2 - wq(y|x)^2) &\geq 0 \\ wy^2 - w^2q(y|x)^2 - y^2 + wq(y|x)^2 + 2wq(y|x)y - 2wq(y|x)y &\geq 0 \\ w(q(y|x) - y)^2 - (wq(y|x) - y)^2 &\geq 0 \end{aligned}$$

□

B EXPERIMENTAL DETAILS

Table 3: Dataset characteristics, where N denotes dataset size and d is the dimensionality.

Dataset	N	d	# of Classes
Ionosphere	351	34	2
Ovarian Cancer	216	4000	2
Heart Disease	303	13	2
Waveform	5000	40	3
Human Activity	10299	561	6
Musk	6598	166	2
CIFAR-10	60000	32×32	10

Units	Description
Init-conv	3×3 conv, 16
Resunit:1-0	3×3 conv, 64 3×3 conv, 64
(Resunit:1-x) \times 4	3×3 conv, 64 3×3 conv, 64 \times 4
(Resunit:2-0)	3×3 conv, 128 3×3 conv, 128
(Resunit:2-x) \times 4	3×3 conv, 128 3×3 conv, 128 \times 4
(Resunit:3-0)	3×3 conv, 256 3×3 conv, 256
(Resunit:3-x) \times 4	3×3 conv, 256 3×3 conv, 256 \times 4
Average Pool	
Fully Connected - 10 logits	

Table 4: 18 unit Complex Model with 15 ResNet units.

Table 5: Residual Network Model used as the complex model for CIFAR-10 experiments in Section 4.2

Simple Model IDs	Additional Resunits	Rel. Size
SM-3	None	$\approx 1/5$
SM-5	(Resunit:1-x) \times 1 (Resunit:2-x) \times 1	$\approx 1/3$
SM-7	(Resunit:1-x) \times 2 (Resunit:2-x) \times 1 (Resunit:3-x) \times 1	$\approx 1/2$

Table 6: Additional Resnet units in the Simple Models apart from the commonly shared ones. The last column shows the approximate size of the simple models relative to the complex neural network model in the previous table.

B.1 ADDITIONAL TRAINING DETAILS

CIFAR-10 Experiments

Complex Model Training: We trained with an ℓ_2 weight decay rate of 0.0002, sgd optimizer with Nesterov momentum (whose parameter is set to 0.9), 600 epochs and batch size 128. Learning rates are according to the following schedule: 0.1 till 40k training steps, 0.01 between 40k-60k

Probes	1	2	3	4	5	6	7	8	9
Training Set 2	0.298	0.439	0.4955	0.53855	0.5515	0.5632	0.597	0.6173	0.6418
Probes	10	11	12	13	14	15	16	17	18
Training Set 2	0.66104	0.6788	0.70855	0.7614	0.7963	0.82015	0.8259	0.84214	0.845

Table 7: Probes at various units and their accuracies on the training set 2 for the CIFAR-10 experiment. This is used in the ProfWeight algorithm to choose the unit above which confidence scores needs to be averaged.

training steps, 0.001 between $60k - 80k$ training steps and 0.0001 for $> 80k$ training steps. This is the standard schedule followed in the code by the Tensorflow authors². We keep the learning rate schedule invariant across all our results.

Simple Models Training:

1. **Standard:** We train a simple model as is on the training set 2.
2. **ConfWeight:** We weight each sample in training set 2 by the confidence score of the last layer of the complex model on the true label. As mentioned before, this is a special case of our method, ProfWeight.
3. **Distilled-temp- t :** We train the simple model using a cross entropy loss with soft targets. Soft targets are obtained from the softmax outputs of the last layer of the complex model (or equivalently the last linear probe) rescaled by temperature t as in distillation of Geoffrey Hinton (2015). By using cross validation, we pick two temperatures that are competitive on the validation set ($t = 0.5$ and $t = 40.5$) in terms of validation accuracy for the simple models. We cross-validated over temperatures from the set $\{0.5, 3, 10.5, 20.5, 30.5, 40.5, 50\}$. See Figures 4 and 5 in the supplementary material for validation and test accuracies for SM-9 model with distillation at different temperatures.
4. **ProfWeight ($\geq \ell$):** Implementation of our ProfWeight algorithm where the weight of every sample in training set 2 is set to the averaged probe confidence scores of the true label of the probes corresponding to units above the ℓ -th unit. We set $\ell = 13, 14$ and 15 . The rationale is that unweighted test scores of all the simple models in Table 2 are all below the probe precision of layer 16 on training set 2 but always above the probe precision at layer 12. The unweighted (i.e. Standard model) test accuracies from Table 2 can be checked against the accuracies of different probes on training set 2 given in Table 5 in the supplementary material.
5. **SRatio:** We average confidence scores from $\ell = 13, 14$ and 15 as done above for ProfWeight and divide by the simple models confidence. In each case, we optimize over β which is increased in steps of 0.5 from 1.5 to 10.

²Code is taken from:
<https://github.com/tensorflow/models/tree/master/research/resnet>.