Identifying Wrongly Predicted Samples: A Method for Active Learning

Rahaf Aljundi  Nikolay Chumerin  Daniel Olmeda Reino
Toyota Motor Europe

Abstract
State-of-the-art machine learning models require access to significant amount of annotated data in order to achieve the desired level of performance. While unlabelled data can be largely available and even abundant, annotation process can be quite expensive and limiting. Under the assumption that some samples are more important for a given task than others, active learning targets the problem of identifying the most informative samples that one should acquire annotations for. Instead of the conventional reliance on model uncertainty as a proxy to leverage new unknown labels, in this work we propose a simple sample selection criterion that moves beyond uncertainty. By first accepting the model prediction and then judging its effect on the generalization error, we can better identify wrongly predicted samples. We further present an approximation to our criterion that is very efficient and provides a similarity based interpretation. In addition to evaluating our method on the standard benchmarks of active learning, we consider the challenging yet realistic scenario of imbalanced data where categories are not equally represented. We show state-of-the-art results and better rates at identifying wrongly predicted samples. Our method is simple, model agnostic and relies on the current model status without the need for re-training from scratch.

1 Introduction
The success of deep learning relies on the availability of large annotated data in which models trained on millions of samples can exceed human level performance in certain tasks (Peter Eckersley et al. 2017), however, obtaining annotations for new data can be a time consuming and a very expensive procedure. Besides, in many applications, e.g., semantic segmentation, samples are not equally important for the task being learned. Many samples can be redundant or easily predicted and annotating them can be a waste of resources. With the goal of improving the data labelling efficiency, active learning is a sub-field of machine learning that aims at identifying the most informative data points in a stream or a large pool of unannotated samples. Those identified samples are then sent for annotation and added to the existing training data, which would contribute to a substantial performance gain upon re-training, a process that can be repeated until reaching a certain level of performance or consuming the annotation budget. While a large body of research has been dedicated to active learning (see Settles 2009 for a survey), fewer research works have considered active learning with deep models. Neural network based methods for selecting labelling candidates can either rely on the uncertainty in their current predictions (Gal and Ghahramani 2016; Wang et al. 2016; Gal, Islam, and Ghahramani 2017) or on how representative the selected candidates are to the rest of the samples (Sener and Savarese 2017), or, alternatively, how different selected samples are from the current training data (Sinha, Ebrahimi, and Darrell 2019). The last two methods (Sinha, Ebrahimi, and Darrell 2019; Sener and Savarese 2017) show state-of-the-art results when extracting large batches of samples from balanced pools of unannotated data. However, the first requires solving a mixed integer optimization problem over all pool samples and the later trains a VAE and a discriminator on the pool and training samples prior to the selection process. In this work, we are interested in developing a lightweight sample selection method, this has its advantage in scenarios with large abundant unlabelled data.

Given this state of mind, the most attractive direction, on one hand, seems to be the uncertainty based approach. On the other hand, this approach requires to train a Bayesian neural network or at least training a network with dropout which might not always be applicable or favorable. In this work, we propose a model agnostic and simple method to select most informative samples. We suggest that informative samples are those that the current trained model has predicted their output (label) wrongly and by acquiring their true labels, the model will gain access to new bits of knowledge. Now the question we aim at answering is if there is a better way of pointing at wrongly predicted samples other than the uncertainty in their predictions. We propose to identify those wrongly predicted samples by first hypothesizing that the model prediction is correct and attempt at increasing the confidence of the model in its initial prediction. We then measure the effect of this hypothesis on the model performance on a small holdout set. As increasing the confidence on wrong predictions would harm the model performance in contrary to correct predictions, we use the relative change in the model performance (or alternatively the error) as a criterion for selecting samples that are likely to be wrongly predicted. Our method is generic,
Aside from these aspects, in this work, we point at the fact that active learning methods have been mostly tested in settings where the pool of unannotated samples is artificially balanced over the different categories as in the case of most standard datasets. This assumption is unrealistic in many cases and hides the potential of the different approaches, e.g., random sampling is only outperformed by a small margin. We argue that real-life applications often face the problem of imbalanced set of samples and the condition where samples are balanced among different classes is solely met in existing benchmarks. In this paper, we consider the challenging setting of imbalanced pool of unannotated samples where not all categories are equally represented. We show that random selection is no longer a competitive baseline and requires significant extra amount of annotations in comparison to our method which targets regions where most mistakes occur and surpasses the imbalanced nature of the data. While our proposed method has a comparable or better performance to its counterparts on the controlled balanced setting, we show a significant improvement on the more realistic scenario of imbalanced pool samples.

Our contributions are as follows: 1) we propose a novel approach for sample selection based on their plausibility of being wrongly predicted by the current trained model. 2) We present an approximated variant of our method and demonstrate an interesting link with kernel based similarity measures, here from a network perspective. 3) We achieve state-of-the-art results especially on the realistic yet challenging imbalanced setting. In the following, we discuss closely related works in Section 2 and describe our proposed approach in Section 3. We evaluate our method on image classification problem, Section 4.1 and semantic segmentation problem, Section 4.2 we conclude in Section 5.

2 Related Work

Active learning is an important field of machine learning and has been studied extensively well before the success of deep learning, we refer to (Settles 2009) [5] for surveys. Our work considers pool based setting where annotation candidates are to be selected from a big pool of unlabelled data. Under this setting, most studied lines of work focus either on identifying current uncertain samples or alternatively a set of diverse and representative samples (Fu, Zhu, and Li 2013). However, our work comes closest to approaches that aim at selecting samples which would, once annotated, incur the largest effect on the trained model. We mention the largest expected model change approach as in EGL (Settles, Craven, and Ray 2008) where samples are selected based on an approximation to the expected value of the sample gradient given the current predicted output distribution. Samples with largest gradient magnitude are selected for annotation. In our method approximation, we don’t depend only on the gradients magnitudes, but also on the angle between the gradient of the pool sample and estimated gradient of the holdout set.

Instead of estimating the model change by the exact gradient length, variance reduction methods (Hassanzadeh and Keyvanpour 2011) [6] aim at implicitly reducing the generalization error by selecting candidates that would minimize the model output variance through the reliance on Fisher information. Closer to our approach, expected error reduction methods, estimate explicitly how much the generalization error is going to be reduced as in (Roy and McCallum 2001). For each candidate, the model is trained on each possible label and the generalization error is computed on other pool samples, approximated with the current model output distribution and further averaged over the different possible labels of the candidate. In our work, we also aim at reducing the generalization error of the model when the selected samples are correctly annotated, however, we select samples that affect most negatively the generalization error when using their current predicted labels as groundtruth. We use this as a proxy to identify wrongly predicted labels. Aside from the novel deployed criterion, in this work, we introduce a series of steps to make such approach applicable to deep learning. Instead of estimating an expectation of the loss on the pool set, we deploy the typically required validation set to estimate the generalization error and instead of estimating the excepted updated model given all possible labels we rely on pseudo labels. More importantly we present an efficient approximation and show how our criterion can be interpreted as selecting samples that are dissimilar to those in the holdout set.

When considering active learning methods designed for deep learning, several paradigms have emerged such as uncertainty based sampling (Gal and Ghahramani 2016, Gal, Islam, and Ghahramani 2017, Kendall and Gal 2017), representation based sampling (Sener and Savarese 2017, Sinha, Ebrahimi, and Darrell 2019) and query by committee using ensemble of models (Gilad-Bachrach, Navot, and Tishby 2006, Seung, Opper, and Sompolinsky 1992). Uncertainty based methods are the most similar in nature to our approach. Gal et al. in (Gal and Ghahramani 2016) showed that MC-Dropout can be used to perform approximate Bayesian inference in deep neural networks, and applied it to high-dimensional image data in (Kendall and Gal 2017) to estimate uncertainty as a selection criterion. Our approach moves beyond uncertainty by selecting samples that are likely to be wrongly predicted using the change in generalization error. In (Wang et al. 2016) the obtained annotations of uncertain samples and the pseudo labels of the most certain samples were combined. In our work, we provide a ranking of the samples, where the points that reduce generalization error can be deployed along with their pseudo labels for further performance improvement. Very recently, (Ash et al. 2019) proposes to rely on the gradient magnitude as a measure of uncertainty while selecting diverse candidates. In our approximation, we select samples that are dissimilar to a holdout set in the gradient space.

3 Our Approach

While standard supervised machine learning methods have access to all available training data for a given task before the start of the learning process, active learning methods assume access to only small initial set $X^i$ of labelled training data along with a much larger set of unannotated data $X^p$ (pool). The active learning method $M$ should identify a set of $K$ most informative samples $X^*$ to be annotated and added to
Pool

Assume that the predicted label is correct, then maximizing work, we propose a new method to spot wrong predictions.

The goal is to estimate each pool sample’s utility, which is about a sample and yet predicts its output correctly. In this mistakes. While a popular line of works (Gal and Ghahramani 2016; Wang et al. 2016; Gal, Islam, and Ghahramani 2017) rely on uncertainty, we argue that a model can be uncertain about a sample and yet predicts its output correctly. In this work, we propose a new method to spot wrong predictions.

We consider a standard classification problem, where the target class $y$ is estimated from the model output $f(x; \theta)$. Starting from the initial predictions of the model, the entropy of these predictions can be used as a measure of uncertainty. Minimizing this entropy, which is usually deployed in unsupervised or semi-supervised learning (Grandvalet and Bengio 2005; Berthelot et al. 2019; Guerrero-Curíeses and Cid-Sueiro 2000), would push the prediction towards the most probable label and suppress other labels probabilities. Assume that the predicted label is correct, then maximizing the confidence in this prediction through maximizing the log-likelihood of the predicted label or alternatively minimizing the cross-entropy loss using the first predicted label as a pseudo label could help improving the model performance. However, if the initial model prediction is wrong then minimizing the loss on a wrong label could harm the model performance as we are injecting false information in the model. We use this reasoning as a base for designing a measure to select wrongly predicted samples. Figure 1 illustrates the main idea behind our approach.

Formally, for each candidate sample $x^p_i \in X^p$, we first obtain its prediction $\hat{y}_i$ by the current model (with $\theta = \theta^*$). In unsupervised learning methods, $\hat{y}_i$ can be seen as a pseudo label and used to train the model (Lee 2013). Here, we first assume that the prediction given by the pseudo label $\hat{y}_i$ is correct and through minimizing the loss $\ell$ on the current sample $x_i^p$ given the pseudo label $\hat{y}_i$ we obtain $\theta^p_i$ as:

$$\theta^p_i = \arg \min \theta \ell (f(x^p_i; \theta), \hat{y}_i).$$

Here $\arg \min \theta \ell (f(x^p_i; \theta), \hat{y}_i)$ denotes the argument-result of the local minimization w.r.t. $\theta$ starting from $\theta^*$. Now, as explained earlier, our hypothesis suggests that if the current model prediction is wrong, the minimization of the model loss given that prediction as a target label would harm the model performance. This can be due to moving the decision boundary in the wrong direction or relying on a feature that is apparent or representative of another category. We use this rule as a proxy to identify the samples that are likely to be wrongly predicted. We propose to select samples using the estimate of the change in the model generalization error, i.e., the change in the model prediction error on unseen samples:

$$S(x^p_i) = \ell (f(X^p_i; \theta^p_i), Y^p) - \ell (f(X^p_i; \theta^*), Y^p).$$

To measure the generalization error, we employ a small set $X^\ast$, this can be a small holdout set or the validation set used for setting hyper-parameters and estimating the model performance. We then select $K$ samples with largest values of $S$ and request their annotations. The newly labelled data are to be added to the training set on which the model will be trained again and then a new active learning step can be carried out. It can be noted that in general the last $K$ samples whose updated model loss decreases are likely to be correctly predicted by the current model and can be combined with the training pool to be learned in an "unsupervised" manner. To summarize, instead of relying only on the model uncertainty to find the annotation candidates, we use the change in the generalization error on a holdout set to identify the wrongly predicted samples.
3.1 First Order Approximation

Our criterion involves estimating the updated model loss on a holdout set after the loss minimization on each pool sample given its pseudo label. As we shall see in the experiments, the holdout set can be very small and its loss can be estimated in one forward pass. Nonetheless, to account for scenarios with extreme constraints on computational cost and more importantly to gain better insights on our proposed method behaviour, we analyse and present an approximation to the selection criterion in (3). Let’s define:

\[ \ell_v(\theta) = \ell(f(X^v; \theta), Y^v) = \sum_j \ell(f(x_j^v; \theta), y_j^v). \] (4)

Then (3) can be rewritten as follows:

\[ S(x_i^p) = \ell_v(\theta^p) - \ell_v(\theta^s). \] (5)

We expand the first term about \( \theta^s \) using first order Taylor series approximation.

\[ \ell_v(\theta^p) \approx \ell_v(\theta^s) + \nabla_\theta \ell_v(\theta^s) \cdot (\theta^p - \theta^s), \] (6)

where \( \nabla_\theta \ell_v(\theta^s) \) denotes the gradient of \( \ell_v(\theta) \) w.r.t. the parameter \( \theta \) at point \( \theta = \theta^s \). Instead of doing full optimization of the loss (mentioned in (3)), we propose to estimate \( \theta^p \) by a single step of gradient descent from \( \theta^s \) with a learning rate \( \eta \) and the loss gradient estimated at sample \( x_i^p \):

\[ \theta^p_i \approx \theta^s - \eta \nabla_\theta \ell(f(x_i^p; \theta^s), \hat{y}_i). \] (7)

Then, using this estimate in the right-hand part of (6), we obtain:

\[
\ell_v(\theta^p_i) \approx \ell_v(\theta^s) + \nabla_\theta \ell_v(\theta^s) \cdot (\theta^p_i - \theta^s - \eta \nabla_\theta \ell(f(x_i^p; \theta^s), \hat{y}_i)) - \ell_v(\theta^s) = -\eta \nabla_\theta \ell_v(\theta^s) \cdot \nabla_\theta \ell(f(x_i^p; \theta^s), \hat{y}_i).
\] (8)

\[
S(x_i^p) \approx \ell_v(\theta^s) - \eta \nabla_\theta \ell_v(\theta^s) \cdot \nabla_\theta \ell(f(x_i^p; \theta^s), \hat{y}_i) - \ell_v(\theta^s) = -\eta \nabla_\theta \ell_v(\theta^s) \cdot \nabla_\theta \ell(f(x_i^p; \theta^s), \hat{y}_i).
\] (9)

The positive constant \( \eta \) in (9) has no influence on the order of \( x_i^p \) sorted by decreasing \( S(x_i^p) \), and, therefore, can be simply dropped. We propose the following alternative criterion and consider both criteria in the experiment Section 4.1.

\[ S_u(x_i^p) = -\nabla_\theta \ell_v(\theta^s) \cdot \nabla_\theta \ell(f(x_i^p; \theta^s), \hat{y}_i). \] (10)

The estimation of the selection criterion \( S_u(x_i^p) \) does not involve the loss minimization of (2) as in the original criterion \( S(x_i^p) \), but uses only the estimation of the pool sample gradient. It also replaces the estimation of the holdout set loss in (3) for each pool sample with a single prior computation of the loss gradient on the holdout set.

A Similarity Based Interpretation. Here we want to present our criterion as a measure of dissimilarity between a given pool sample and samples of the holdout set based on the currently trained model. Let’s define the following kernel:

\[ K_\theta(x_i, x_j) = \nabla_\theta \ell(f(x_i; \theta), y_i) \cdot \nabla_\theta \ell(f(x_j; \theta), y_j). \] (11)

Each term in (11) can be expanded using chain rule as follows:

\[
\nabla_\theta \ell(\theta) = (\nabla_\theta f(x_i; \theta))^T \ell',
\]

where \( \ell' \in \mathbb{R}^C \) denotes the derivative of \( \ell \) w.r.t. \( f(x_i; \theta) \), and \( \nabla_\theta f(x_i; \theta) \in \mathbb{R}^{C \times P} \) with \( C \) the number of categories and \( P \) the size of the parameter vector. The kernel can be written as follows:

\[ K_\theta(x_i, x_j) = (\nabla_\theta f(x_i; \theta))^T \ell' \cdot (\nabla_\theta f(x_j; \theta))^T \ell'. \] (12)

This kernel is related to the Neural Tangent Kernel (NTK) (Jacot, Gabriel, and Hongler 2018), \( K \text{NTK} (x_i, x_j) = \nabla_\theta f(x_i; \theta) \cdot \nabla_\theta f(x_j; \theta) \), studied from an optimization point of view in the infinite width limit, and describes how changing the network function at one point would affect its output on another. A kernel similar to NTK was proposed in (Chapati et al. 2019) to measure the similarity between samples from a trained network perspective for dataset self denoising. In the same study it was shown that \( \nabla_\theta f(x_i; \theta) = \nabla_\theta f(x_j; \theta) \) follows \( f(x_i; \theta) = f(x_j; \theta) \), and samples with dissimilar features have orthogonal gradient directions and kernels value close to zero. The kernel, defined in (13), considers additionally the gradient of the loss function accounting for the sample/label pair. For example, in the case of a cross-entropy loss, we have \( K_\theta(x_i, x_j) = (\nabla_\theta f(x_i; \theta))^T (p_i - y_i) \cdot (\nabla_\theta f(x_j; \theta))^T (p_j - y_j) \) with \( y_i \) here constructed as a one-hot label vector and \( p_i \) the output probability, which can be seen as weighting the function gradient by the difference between the predicted class probabilities and the target/pseudo labels. See supplementary materials for details on the derivation. Finally, given that \( \nabla_\theta \ell_v(\theta) = \sum_i \nabla_\theta \ell(f(x_i^p; \theta), y_i^p) \) where \( j \) is the index of the holdout samples, our approximated criterion can be rewritten as follows:

\[ S_u(x_i^p) = -\sum_j K_\theta(x_i^p, x_j^p). \] (14)

Following that, our criterion allows to select the samples that are dissimilar to those in the holdout set according to the kernel defined in (11).

Binary classification example. Let us demonstrate the proposed sample selection method on a binary classification problem employing a single-layer neural network parametrized by \( \theta \). Assume the input to the network is a feature vector \( \phi(x) \in \mathbb{R}^p_{\geq 0} \) extracted from a sample \( x \) with a fixed (non-trainable) feature extractor \( \phi \). The function being learned is \( f_0(\phi(x)) = \theta^T \phi(x) \). By defining \( z = f_0(\phi(x)) \), and the loss \( \ell(z, y) = -y \log(\sigma(z)) - (1 - y) \log(1 - \sigma(z)) \), where \( y \in \{0, 1\} \) is the binary label, and \( \sigma(z) = \frac{1}{1 + e^{-z}} \); the gradient of the loss w.r.t. \( \theta \) can be derived using chain rule:

\[
\nabla_\theta \ell(z, y) = \frac{\partial \ell(z, y)}{\partial \theta} = \frac{\partial \ell}{\partial \sigma} \frac{\partial \sigma}{\partial z} \frac{\partial z}{\partial \theta} = (\sigma(z) - y) \phi(x).
\]

(15)

Following this definition, our criterion for selecting pool samples is:

\[ S_u(x_i^p) = -\sum_j (\sigma(z_i^p) - y_i) \phi(x_i) \cdot (\sigma(z_j^p) - y_j) \phi(x_j^p). \] (16)

Let us analyze the kernel value w.r.t. a pool sample \( x_i^p \) and a sample from the holdout set \( x_j^p \):

\[ K_\theta(x_i^p, x_j^p) = c \phi(x_i^p) \cdot \phi(x_j^p), \text{ with scalar } c = (\sigma(z_i^p) - y_i) (\sigma(z_j^p) - y_j). \] (17)
Consider the following cases: 1) the feature vectors \( \phi(x_i^p) \) and \( \phi(x_j^p) \) are different and \( \phi(x_i^p) \cdot \phi(x_j^p) = 0 \), resulting in \( K_\theta(x_i^p, x_j^p) \approx 0 \); 2) \( x_i^p \) and \( x_j^p \) are close in the feature space and \( \phi(x_i^p) \cdot \phi(x_j^p) \gg 0 \). In the latter case, either \( \hat{y}_i \neq y_j^p \) and \( c < 0 \), causing \( K_\theta(x_i^p, x_j^p) \ll 0 \) (case 2a), or \( \hat{y}_i = y_j^p \) and \( c > 0 \), leading to \( K_\theta(x_i^p, x_j^p) \gg 0 \) (case 2b). Therefore, if \( x_i^p \) differs significantly from all holdout samples (case 1), then \( S_\nu(x_i^p) \approx 0 \). However, if \( x_i^p \) is similar to some holdout samples and it is predicted incorrectly (case 2b), then \( S_\nu(x_i^p) \) is likely to be positive, otherwise, when the prediction is correct (case 2b), the corresponding \( S_\nu(x_i^p) \) is likely to be negative. Consequently, the pool samples from both former cases would get greater (than the samples from the later case) values of the selection criterion and, therefore, will be selected for annotation.

In a nutshell, our method aims at selecting pool samples that differ from the holdout samples firstly in their (probably wrongly) predicted label or in their feature representation.

4 Experiments

To evaluate the effectiveness of our approach in various active learning scenarios, we perform a wide set of experiments on both image classification (Section 4.1), and image segmentation (Section 4.2).

4.1 Image Classification

We first compare our proposed method and its first order approximation with state-of-the-art methods on the standard setting where datasets are balanced and all categories are represented equally. We then move to a closer simulation of real life applications where we construct an active learning benchmark with imbalanced pool and initial training data.

Datasets. On both settings we consider MNIST (LeCun et al. 1998) dataset for handwritten digit recognition, KMNIST (Clanuwat et al. 2018) an MNIST style dataset for Kanji characters composed of 10 classes, SVHN (Netzer et al. 2011) Google street view house numbers dataset and Cifar10 (Krizhevsky, Hinton et al. 2009).

Compared methods. - Random: a random subset of the pool is selected for annotation at each step.
- Err-Reduction (Roy and McCallum 2001): an implementation of the error reduction approach using pseudo labels and error estimation on subset of the pool.
- MC-Dropout (Gal and Ghahramani 2016): uses as a criterion the model uncertainty of each pool sample.
- Coreset (Sener and Savarese 2017): selects a set of representative samples covering the rest of the pool. The method presents a mixed integer programming solution and a greedy alternative that is only 1–2% inferior, we employ this efficient alternative.
- BALD (Gal, Islam, and Ghahramani 2017): it is based on the mutual information between the prediction and the model posterior.
- BADGE (Ash et al. 2019) selects diverse and uncertain samples in a gradient space based on the pseudo labels of pool samples.

Implementation. We deploy a two-layer fully connected network for MNIST and KMNIST datasets, and ResNet18 for SVHN and Cifar10. All methods were trained using ADAM with early stopping on the validation set. We don’t retrain the model from scratch after each annotation step, we rather continue training the model and only reset the optimizer parameters. This makes more sense since the new samples are selected based on a criterion linked to the previously trained model. We apply this to all methods and observe consistent improvement. For our method, we consider both the criterion in (3) and refer to it as Ours, and the first order approximation criterion in (10) and refer to it as Ours-app. We use the initial validation set as a holdout set to estimate the criterion of both Ours and Ours-app. Note that in our experiments we keep the validation set fixed to the initial setting while in practice one can augment it as new labels are obtained. We limit the optimization of the loss in (9) to the last layer parameters and similarly for the gradients estimation of (10) of Ours-app criterion. This has a valuable advantage computationally and shows no significant effect on the performance, see supplementary materials. The minimization of (9) in Ours is performed with SGD and limited to 3 iterations with learning rate \( \eta = 10^{-3} \) on the fully connected model and \( \eta = 10^{-4} \) on ResNet. We report the average of 10 runs with different random seeds along with the standard deviation.

Balanced Setting. The used datasets are standard datasets in the field and they are composed of similar number of samples for each category. As such, the pool and the randomly sampled initial training set represent equally each category. We refer to this setting as balanced setting. Here, we use a validation set of the same size as the initial training set. Each active learning round is composed of 10 annotation steps with each step being 10% of the initial training set size. The initial training set size is relative to each dataset difficulty and the amount of samples needed to obtain a reasonable initial performance. We use the following initial sizes 50, 100, 500, 5000 for MNIST, KMNIST, SVHN and Cifar10 respectively. Figures 2a, 2b, 2c and 3a report the accuracy of each of the compared methods after each annotation step on MNIST, KMNIST, SVHN and Cifar10 datasets respectively. See supplementary materials for more results. While most methods improve over random sampling, the margin of improvement is limited (2%–3%). When considering all the studied datasets, Ours and Ours-app performs similarly to BALD, MC-Dropout, Err-Reduction and BADGE. It is worth noting that Ours-app is the fastest to compute, as discussed in supplementary.

Imbalanced Setting. In the standard balanced setting, Random appears to be a competitive baseline and only outperformed by a small margin as also shown in (Sinha, Ebrahimi, and Darrell 2019). Here, we argue that random sampling cannot be taken for granted as a competitive method in the cases where there are dominant categories that are not of much importance to the task at hand as opposed to the under-represented ones. For example, in autonomous driving applications most images contain examples of road, sky or buildings, but other categories like cyclists or trains are much less frequent. We simulate this scenario by constructing a pool of samples in which half of the categories are under-
represented with number of samples equals to 1/10 of other categories samples (base number of samples per class). Since the compared methods start with initial training set, we also construct this set with the same imbalanced setting. Regarding the validation set, we keep it balanced but limit its size to 1/5 of the initial training size. We apply this setup to the 4 studied datasets. As this is a much harder setting, for each dataset we double the base class size of the initial training set compared to the expected per category size in balanced setting, we also double the annotation step size.

Figures 3a, 3b, 3c, 4b report the accuracy of each of the compared methods after each annotation step on the imbalanced sets of MNIST, KMNIST, SVHN and Cifar10 respectively, see supplementary materials for more results. This setting shows larger differences between the compared methods. It is clear that Random baseline fails to compete here, for example, on MNIST Ours with only 5 annotation steps achieves the same accuracy of Random after 10 annotation steps. This is a reduction of half of the annotation resources. Uncertainty and information based methods BAuLD, BADGE and MC-Dropout continue to improve over Random with a larger margin in this setting. Corest, in the contrary, has consistently lower performance, we think that this method is more suitable for extracting much larger batches of data. Ours achieves the best performance on MNIST, KMNIST and SVHN settings with a substantial margin. We believe that this is a significant improvement that shows our method ability to identify those underrepresented categories where most mistakes occur, and thereof selects most informative samples contributing to higher gains in the trained model performance. Notably, Ours is constantly outperforming Err-Reduction. This indicates that using the largest generalization error as a proxy for identifying wrongly predicted samples provides the model with previously unknown knowledge and results in a larger reduction of the newly trained model generalization error than when aiming at explicitly reducing it.

For Cifar10 dataset, all methods perform closely; we think it is due to the low intra class similarity of this dataset which reduces the potential impact of the individual selected samples. Ours-app improves over other methods on MNIST, KMNIST and SVHN benchmarks with slightly less margin than Ours and achieves comparable performance on Cifar10. This is also important results given its low complexity.

**Holdout Set Size.** Our criterion is based on the generalization error of the model \( f(x; \theta) \), for \( \theta = \theta_i \) – the updated parameters of each pool sample, and depends on the used holdout set, regarded as representative of the different concepts (categories). In all experiments, we have used the validation set for estimating our selection criterion. For the imbalanced setting, the validation set was uniformly sampled but significantly smaller than the size of the initial training set. In this paragraph, we study empirically the effect of the holdout set size on the behaviour of our method. Given an MLP backbone, \( \theta \) shows the performance of Ours using different holdout set sizes on imbalanced MNIST, see sup-
Mistakes Selection. Our approach aims at better identifying the wrongly predicted pool samples, which, once annotated, should improve the model performance, as it is being trained on previously unknown cases. We inspect the percentage of samples with wrong predictions in comparison to BALD and MC-Dropout as their criteria are related to the purpose of Ours. Table 1 reports the accuracy in mistake selection at the indicated steps in MNIST balanced setting. Both our criteria are best at picking wrongly predicted samples, with Ours achieving a higher mistake selection rate, 10%–20%, than others. This behaviour was consistent on different settings/datasets. It further shows that our method outperforms the typical use of uncertainty and identifies better samples that are likely to be wrongly predicted.

4.2 Semantic Segmentation Experiments

In the previous experiments, each sample has only one possible true class. We are interested in the case where each sample contributes to multiple and possibly conflicting hypotheses, thus we consider semantic segmentation.

We mainly compare to Random and MC-Dropout described previously, Section 4.1. For Ours and Ours-app: we only optimize the parameters or compute the gradients on the last two convolutional layers. We adapt Ours to the case where an imperfect model produces both correct and incorrect predictions for one sample. We average pixel predictions (3), where \( \ell(f(X^c; \theta^c), Y^c) > \ell(f(X^i; \theta^c), Y^i) \) holds, and by doing so we only consider the subset of the frame that indicates that the model has been negatively impacted by the pool sample. See supplementary for further details and results. Fig. 4c shows the mean Intersection over Union (mIoU) after each annotation step. Ours and MC-Dropout perform closely, with Ours having slightly higher mIoU scores towards the end.
5 Conclusion

We propose a new solution to the problem of active learning that first accepts the hypothesis of the current model prediction on each pool sample and then judges the effect of increasing this hypothesis confidence on the performance on a holdout set. We use the change in the model generalization error as an indication of how likely the prediction of a given sample is to be mistaken. We further develop an approximation of our selection criterion and show that it targets sample/prediction pairs that are dissimilar to those in the holdout set from the current model perspective. We evaluate our approach on several benchmarks and achieve comparable performance to state-of-the-art methods. Additionally, we setup for the first time a systematic compassion on the important and realistic imbalanced setting where we show significant improvements. Our method is computationally efficient and requires no changes on the available model.

Ethical Impact

In general terms, active learning methods serve as enablers of machine learning models, and thus inherit similar ethical implications, perhaps accentuated by faster learning cycles. Other than the purpose and the ultimate application of the machine learning model, active learning can potentially have an impact on the use of data, and on human annotators. Regarding the latter, active learning aims at optimizing knowledge transfer from human experts to machine learning models, by directing attention to potentially meaningful samples. The implication would be that fewer resources are needed to achieve a task that sometimes may be considered as tedious and repetitive, but also that knowledge from those experts may eventually become irrelevant, as their expertise is superseded by that of the collectively annotated data. As for the use of data, active learning methods, such as the one proposed in this work, are relevant to alleviate biases introduced in the data pool by an imperfect data collection process, or by the unbalanced nature of the true distribution of the data.

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