Active Testing: Sample–Efficient Model Evaluation

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Abstract

We introduce a new framework for sample-efficient model evaluation that we call active testing. While approaches like active learning reduce the number of labels needed for model training, existing literature largely ignores the cost of labeling test data, typically unrealistically assuming large test sets for model evaluation. This creates a disconnect to real applications, where test labels are important and just as expensive, e.g. for optimizing hyperparameters. Active testing addresses this by carefully selecting the test points to label, ensuring model evaluation is sample-efficient. To this end, we derive theoretically-grounded and intuitive acquisition strategies that are specifically tailored to the goals of active testing, noting these are distinct to those of active learning. As actively selecting labels introduces a bias; we further show how to remove this bias while reducing the variance of the estimator at the same time. Active testing is easy to implement and can be applied to any supervised machine learning method. We demonstrate its effectiveness on models including WideResNets and Gaussian processes on datasets including Fashion-MNIST and CIFAR-100.

1. Introduction

Although unlabeled datapoints are often plentiful, labels can be expensive. For example, in scientific applications acquiring a single label can require expert researchers and weeks of lab time. However, some labels are more informative than others. In principle, this means that we can pick the most useful points to spend our budget wisely.

These ideas have motivated extensive research into actively selecting training labels (Atlas et al., 1990; Settles, 2010), but the cost of labeling test data has been largely ignored.

(Atlas et al., 1990). In artificial research settings, this is often not a problem: we can ‘cheat’ by using enormous test datasets if the goal is to see how good some sample-efficient training approach is. But for practitioners this creates a huge issue: in practice, one must evaluate model performance, both to choose the best model and to develop trust in individual models. Whenever labels are expensive enough that we need to carefully pick training data, we cannot afford to be wasteful with test data either.

To address this, we introduce a framework for actively selecting test points for efficient labeling that we call active testing. To this end, we derive acquisition functions with which to select test points to maximize the accuracy of the resulting empirical risk estimate. We find that the principles that make these acquisition functions effective are quite different from their active learning counterparts. Given a fixed budget, we can then estimate quantities like the test loss much more accurately than naively labeling points at random. An example of this is given in Fig. 1.

Starting with an idealized, but intractable, approach, we show how practical acquisition strategies for active testing can be derived. In particular, we derive specific principled acquisition frameworks for classification and regression. Each of these depends only on a predictive model for outputs, allowing for substantial customization of the framework to particular problems and computational

Figure 1. Active testing estimates the test loss much more precisely than uniform sampling for the same number of labeled test points. Active data selection during testing resolves a major barrier to sample-efficient machine learning, complementing prior work which has focused only on training. For details, see §5.1.
Active Testing: Sample–Efficient Model Evaluation

Our goal is to estimate some model evaluation statistic in a sample-efficient way. Depending on the setting, this could be a test accuracy, mean squared error, negative log-likelihood, or something else. For sake of generality, we can write the ‘test loss’ for arbitrary loss functions $\mathcal{L}$ evaluated over a test set $D_{test}$ of size $N$ as

$$\hat{R} = \frac{1}{N} \sum_{i_n \in D_{test}} \mathcal{L}(f(x_{i_n}), y_{i_n}).$$  

(1)

This test loss is an unbiased estimate for the true risk $R = \mathbb{E}[\mathcal{L}(f(x), y)]$ and is what we would be able to calculate if we possessed labels for every point in the test set. However, for active testing, we cannot afford to label all the test data. Instead, we can label only a subset $D_{test}^{observed} \subseteq D_{test}$. Although we could choose all elements of $D_{test}^{observed}$ in a single step, doing so is sub-optimal as information garnered from previously acquired labels can be used to select future points more effectively. Thus, we will pre-emptively introduce an index $m$ tracking the labeling order: at each step $m$, we acquire the label $y_{i_m}$ for the point with index $i_m$ and add this point to $D_{test}^{observed}$.

2.1. A Naive Baseline

Standard practice ignores the cost of labeling the test set—it does not actively pick the test points. For a labeling budget $M$, this is equivalent to uniformly sampling a subset of the test data and then calculating the subsample empirical risk

$$\hat{R}_{iid} = \frac{1}{M} \sum_{i_m \in D_{test}^{observed}} \mathcal{L}(f(x_{i_m}), y_{i_m}).$$  

(2)

Uniform sampling guarantees the data are independently and identically distributed (i.i.d.) so that the estimate is unbiased, $\mathbb{E}[\hat{R}_{iid}] = \hat{R}$, and converges to the empirical test risk, $\hat{R}_{iid} \rightarrow R$ as $M \rightarrow N$. However, although this estimator is unbiased its variance can be high in the typical setting of $M \ll N$. That is, on any given run the test loss estimated according to this method might be very different from $\hat{R}$, even though they will be equal in expectation.

2.2. Actively Sampling Test Points

To improve on this naive baseline, we need to reduce the variance of the estimator. A key idea of this work is that this can be done by actively selecting the most useful test points to label. Unfortunately, doing this naively will introduce unwanted and highly problematic bias into our estimates.

In the context of pool-based active learning, Farquhar et al. (2021) showed that biases from active selection can be corrected by using a stochastic acquisition process and formulating an importance sampling estimator. Namely, they introduce an acquisition distribution $q(i_m)$ that denotes the probability of selecting index $i_m$ to be labeled. They then compute the Monte Carlo estimator $\hat{R}_{LURE}$ which, in
active testing setting, takes the form
\[
\hat{R}_{LURE} = \frac{1}{M} \sum_{m=1}^{M} v_m \mathcal{L}(f(x_{i_m}), y_{i_m}),
\]
where \(M\) is the size of \(D_{\text{test}}^{\text{observed}}\), \(N\) is the size of \(D_{\text{test}}\), and
\[
v_m = 1 + \frac{N - M}{N - m} \left(1 - \frac{1}{(N - m + 1)q(i_m) - 1}\right).
\]
Not only does \(\hat{R}_{LURE}\) correct the bias of active sampling, if the proposal \(q(i_m)\) is suitable it can also (drastically) reduce the variance of the resulting risk estimates compared to both \(R_{\text{ideal}}\) as well as naively applying active sampling without bias correction. This is because \(\hat{R}_{LURE}\) is based on importance sampling: a technique designed precisely for reducing variance through appropriate proposals (Kahn & Marshall, 1953; Kahn, 1955; Owen, 2013).

Importantly, there are no restrictions on how \(q(i_m)\) can depend on the data, and in our context \(q(i_m)\) is actually shorthand for \(q(i_m; t_{i_m-1}, D_{\text{test}}, D_{\text{train}})\). This means that we will be able use proposals that depend on the already acquired test data, as well as the training data and the trained model, as we explain in the next section.

3. Acquisition Functions for Active Testing

In the last section, we showed how to construct an unbiased estimator of the test risk using actively sampled test data. This is exactly the quantity that the practitioner cares about for evaluating a model. For an estimator to be sample-efficient, its variance should be as small as possible for any given number of labels, \(M\). We now use this principle to derive acquisition proposal distributions (i.e. acquisition functions) for active testing by constructing an idealized proposal and then showing how it can be approximated.

3.1. General Framework

As shown by Farquhar et al. (2021), the optimal oracle proposal for \(\hat{R}_{LURE}\) is to sample in proportion to the true loss of each data point, resulting in a single-sample zero-variance estimate of the risk. In practice, we cannot know the true loss before we have access to the actual label. In particular, the true distribution of outputs for a given input is typically noisy and we can never know this noise without evaluating the label. In the context of deriving an unbiased Monte Carlo estimator, the best we can ever hope to achieve is to sample from the expected loss over the true \(y | x_{i_m}\),

\[
q^*(i_m) \propto \mathbb{E}_{p(y|x_{i_m})} [\mathcal{L}(f(x_{i_m}), y)].
\]

Note that as \(i_m\) can only take on a finite set of values, the required normalization can be performed straightforwardly.

Of course, \(q^*(i_m)\) remains intractable because we do not know the true distribution for \(y | x_{i_m}\). We need to approximate it for unlabeled \(x_{i_m}\) in a way that captures regions where \(f(x)\) is a poor predictive model as these will contribute the most to the loss. This can be hard as \(f(x)\) itself has already been designed to approximate \(y|x\).

Thankfully, we have the following tools at our disposal to deal with this: (a) We can incorporate uncertainty to identify regions with a lack of available information (e.g. regions far from any of the training data); (b) We can introduce diversity in our predictions compared to \(f(x)\) (thereby ensuring that mistakes we make are as distinct as possible to those of \(f(x)\)); and (c) as we label new points in the test set, we can obtain more accurate predictions than \(f(x)\) by incorporating these additional points. These essential strategies will help us identify regions where \(f(x)\) provides a poor fit. We give examples of how we incorporate them in practice in §3.4.

We now introduce a general framework for approximating \(q^*(i_m)\) that allows us to use these mechanisms as best as possible. The starting point for this is to consider the concept of a surrogate for \(y|x\), where we introduce some potentially infinite set of parameters \(\theta\), a corresponding generative model \(\pi(\theta)\pi(y|x, \theta)\), and then approximate the true \(p(y|x)\) using the marginal distribution \(\pi(y|x) = \mathbb{E}_{\pi(\theta)} [\pi(y|x, \theta)]\) of the surrogate. We can now approximate \(q^*(i_m)\) as

\[
q(i_m) \propto \mathbb{E}_{\pi(\theta)} \mathbb{E}_{\pi(y|x_{i_m}, \theta)} [\mathcal{L}(f(x_{i_m}), y)].
\]

With \(\theta\) we represent our subjective uncertainty over the outcomes in a principled way. However, our derivations will lead to acquisition strategies also compatible with discriminative, rather than generative, surrogates, for which \(\theta\) will be implicit.

3.2. Illustrative Example

Figure 2 shows how active testing chooses the next test point among all available test data. The model, here a Gaussian process (Rasmussen, 2003), has been trained using the training data and we have already acquired some test points (crosses). Figure 2 (b) shows the true loss known only to an oracle. Our approximate expected loss is a good proxy in some parts of the input space and worse elsewhere. The next point is selected by sampling proportionately to the approximate expected loss. In this example, the surrogate is a Gaussian process that is retrained whenever new labels are observed. The closer the approximate expected loss is to the true loss, the lower the variance of the estimator \(\hat{R}_{LURE}\) will be; the estimator will always be unbiased.

3.3. Deriving Acquisition Functions

We now give principled derivations leading to acquisition functions for a variety of widely-used loss functions.
where the first term is the variance in our mean prediction and represents our epistemic uncertainty and the latter is our mean prediction of the ‘aleatoric variance’ (label noise). This is why our construction using \( \theta \) is crucial: it stresses that (8) should also take epistemic uncertainty into account.

For regression models with Gaussian outputs \( \mathcal{N}(f(x), \sigma^2) \), the negative log-likelihood loss function and the squared error are related by affine transformation—and following (6) so are the acquisition functions.

**Classification.** For classification, predictions \( f(x) \) generally take the form of conditional probabilities over outcomes \( y \in \{1, \ldots, C\} \). First, we study cross-entropy

\[
\mathcal{L}(f(x), y) = -\log f(x)_y, \tag{10}
\]

Here, we again introduce a surrogate, and, using (6), obtain

\[
q(i_m) \propto \mathbb{E}_{\pi(y|x_{im})} \left[ -\log f(x_{im})_y \right]. \tag{11}
\]

Now expanding the expectation over \( y \) yields

\[
q(i_m) \propto -\sum_y \pi(y \mid x_{im}) \log f(x_{im})_y, \tag{12}
\]

which is the cross-entropy between the marginal predictive distribution of our surrogate, \( \pi(y \mid x_{im}) \), and our model.

We can also derive acquisition strategies based on accuracy. Namely, writing one minus accuracy to obtain a loss,

\[
\mathcal{L}(f(x), y) = 1 - 1[y = \arg \max_{y'} f(x)_{y'}], \tag{13}
\]

and substituting into (6) yields

\[
q(i_m) \propto 1 - \pi(y = y^*(x_{im}) \mid x_{im}), \tag{14}
\]

where \( y^*(x_{im}) = \arg \max_{y'} f(x_{im})_{y'} \).

### 3.4. Tactics for Obtaining Good Surrogates

In §3.1 we introduced three ways for the surrogate to assist in finding high-loss regions of \( f(x) \): we want it to (a) account for uncertainty over the outcomes, (b) make predictions that are diverse to \( f(x) \), and (c) incorporate information from all available data. Motivated by this, we apply the following tactics to obtain good surrogates:

**Uncertainty.** We should use surrogates that incorporate both epistemic and aleatoric uncertainty effectively, and further ensure that these are well-calibrated. Capturing epistemic uncertainty is essential to predicting regions of high loss, while aleatoric uncertainty still contributes and cannot be ignored, particularly if heteroscedastic. A variety of different approaches can be effective in this regard and thus provide successful surrogates. For example, Bayesian neural networks, deep ensembles, and Gaussian processes.

**Fidelity.** In real-world settings, \( f \) may be constrained to be memory-efficient, fast, or interpretable. If labels are
expensive enough, we can relax these constraints at test time and construct a more capable surrogate. In fact, we practically find that using an ensemble of models like $f$ is a robust way of achieving sample-efficiency.

**Diversity.** By choosing the surrogate from a different model family or adjusting its hyperparameters, we can decorrelate the errors of the surrogate and $f$, resulting in better exploration. For example, we find that random forests (Breiman, 2001) can help evaluate neural networks.

**Extra data.** If our computational constraints are not critical, we should retrain the surrogate on $\mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{test}}$ after each step. The exposure to additional data will make the surrogate a better approximation of the true outcomes.

**Thompson-Ensemble.** Retraining the surrogate can also create diversity in predictions due to stochasticity in the training process, the addition of new data, or even deliberate randomization. In fact, we can view retraining the surrogate at regular intervals as implicitly defining an ensemble of surrogates, with the surrogate used at any given iteration forming a Thompson-sample (Thompson, 1933) from this ensemble. This will generally be more powerful and more diverse than a single surrogate, providing further motivation for retraining and potentially even deliberate variations in surrogates/hyperparameters between iterations.

In §5 we empirically assess the relative importance of these considerations, which depends heavily on the situation. For example, the benefit of retraining using the labels acquired at test-time is especially large in very low-data settings, while the benefit of ensembling can be large even when there is more data available. Putting everything together, Algorithm 1 provides a summary of our general framework.

If compute is at a premium for acquisitions, a simple alternative heuristic is to use our original model for the surrogate. This avoids learning a new predictive model, but it suffers because now the surrogate can never disagree with $f$. Instead, we have to rely entirely on uncertainties for approximating (6); for regression, $1$ in (8) is zero, and for classification, (12) reduces to the predictive entropy. In general, we do not recommend this strategy, unless computational constraints are substantial and there is reason to believe that the epistemic and aleatoric uncertainties from $f$ represent the true loss well. If the latter is true, this simplistic approach can perform surprisingly well, although it is always outperformed by more complex strategies. In particular, training a single fixed surrogate that is distinct from $f$ will still typically provide noticeable benefits.

### 4. Related Work

Efficient use of labels is a major aim in machine learning and it is often important to use large pools of unlabeled data through unsupervised or semi-supervised methods (Chapelle et al., 2009; Erhan et al., 2010; Kingma et al., 2014).

An even more efficient strategy is to collect only data that is likely to be particularly informative in the first place. Such approaches are known as optimal or adaptive experimental design (Lindley, 1956; Chaloner & Verdinelli, 1995; Sebastiani & Wynn, 2000; Foster et al., 2020; 2021) and are typically formalized through optimizing the (expected) information gained during an experiment.

Perhaps the best-known instance of adaptive experimental design is active learning, wherein the designs to be chosen are the data points for which to acquire labels (Atlas et al., 1990; Settles, 2010; Houlsby et al., 2011; Sener & Savarese, 2018). This is typically done by optimizing, or sampling...

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**Algorithm 1 Active Testing**

**Input:** Model $f$ trained on data $\mathcal{D}_{\text{train}}$

1. Train surrogate $\pi$ & choose acquisition proposal form $q$
2. for $m = 1$ to $M$ do
3. $i_m \sim q(i_m; \pi)$, observe $y_{i_m}$, add to $\mathcal{D}_{\text{observed}}$
4. Calculate $L(f(x_{i_m}), y_{i_m})$ and $\nu_{i_m}$ $\triangleright$ Eq. (4)
5. Update $\pi$, e.g. retraining on $\mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{observed}}$ $\triangleright$ Eq. (3)
6. end for
7. Return $\hat{R}_{\text{LURE}}$ $\triangleright$ Eq. (3)

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**Why are acquisition strategies different for active learning and active testing?**

Researchers have already investigated acquisition functions for active learning, and it would be helpful if we could just apply these here. However, active testing is a different problem conceptually because we are not trying to use the data to fit a model.

First, popular approaches for active learning avoid areas with high aleatoric uncertainty while seeking out high epistemic uncertainty. This motivates acquisition functions like BALD (Houlsby et al., 2011) or BatchBALD (Kirsch et al., 2019). For active testing, however, areas of high aleatoric uncertainty can be critical to the estimate.

Second, as Imberg et al. (2020) point out, the optimal acquisition scheme for active learning will minimize the expected generalization error at the end of training. They show how this motivates additional terms beyond what one would get from minimizing the variance of the loss estimator.

Third, as Farquhar et al. (2021) show, a biased loss estimator can be helpful during training because it often partially cancels the natural bias of the training loss. This is no longer true at test-time, where we want to minimize bias as much as possible.
from, an acquisition function, with much discussion in the literature on the form this should take (Imberg et al., 2020).

What most of this work neglects is the wasteful acquisition of data for testing. Lowell et al. (2019) acknowledge this and describe it as a major barrier to the adoption of active learning methods in practice. The potential for ‘active testing’ was raised by Nguyen et al. (2018), but they focused on the special case of noisily annotated labels that must be vetted and did not acknowledge the substantial bias that their method introduces. Farquhar et al. (2021) introduce the variance-reducing unbiased estimator for active sampling which we apply. However, their focus is mostly on correcting the bias of active learning (Bach, 2007; Sugiyama, 2006; Beygelzimer et al., 2009; Ganti & Gray, 2012) and they do not consider appropriate acquisition strategies for active testing. Note that their theoretical results about the properties of $\hat{R}_{LURE}$ carry over to active setting.

Other methods like Bayesian Quadrature (Rasmussen & Ghahramani, 2003; Osborne, 2010) and kernel herding (Chen et al., 2012) can also sometimes employ active selection of points. Of particular note, Osborne et al. (2012); Chai et al. (2019) study active learning of model evidence in the context of Bayesian Quadrature.

Bennett & Carvalho (2010); Katariya et al. (2012); Kumar & Raj (2018); Ji et al. (2021) explore the efficient evaluation of classifiers based on stratification, rather than active selection of individual labels. Namely, they divide the test pool into strata according to simple metrics such as classifier confidence. Test data are then acquired by first sampling a stratum and then selecting data uniformly within. Sample-efficiency for these approaches could be improved by performing active testing within the strata. Sawade et al. (2010) similarly explore active risk estimation through importance sampling, but rely on sampling with replacement which is suboptimal in pool-based settings (see Appendix D). Moreover, like the other aforementioned works, they do not consider the use of surrogates to allow for more effective acquisition strategies.

5. Empirical Investigation

We now assess the empirical performance of active testing and investigate the relative merits of different strategies. Similar to active learning, we assume a setting where sample acquisition is expensive, and therefore, per-sample efficiency is critical. Full details as well as additional results are provided in the appendix, and we release code for reproducing the results at github.com/jlko/active-testing.

We note a small but important practicality: we ensure all points have a minimum proposal probability regardless of the acquisition function value, to ensure that the weights are bounded even if $q$ is badly calibrated (cf. Appendix B.1).

5.1. Synthetic Data

We first show that active testing on synthetic datasets offers sample-efficient model evaluations. By way of example, we actively evaluate a Gaussian process (Rasmussen & Ghahramani, 2003) and a linear model for regression, and a random forest (Breiman, 2001) for classification. For regression, we estimate the squared error and acquire test labels via Eq. (8); for classification, we estimate the cross-entropy loss and acquire with Eq. (12). We use Gaussian process and random forest surrogates that are retrained on all observed data after each acquisition.

Figure 3 shows how the difference between our test loss estimation and the truth (known only to an oracle) is much smaller than the naive $R_{iid}$: active testing allows us to precisely estimate the empirical test loss using far fewer samples. For example, after acquiring labels for only 5 test points in (a), the standard deviation of active testing is already as low as it is for i.i.d. acquisition at step 40, nearly the entire test set. Further, we can see that the estimates of $R_{LURE}$ are indeed unbiased. Appendix A.1 gives experiments on additional synthetic datasets.
Radial BNN on MNIST
ResNet-18 on Fashion-MNIST

Figure 4. Median squared errors for (a) Radial BNN on MNIST and (b) ResNet-18 on Fashion-MNIST in a small-data setting. Original Model samples proportional to predictive entropy, X Surrogate iteratively re-trains a surrogate on all observed data, and ResNet Train Ensemble is a deep ensemble trained on \( D_{\text{train}} \) once. Lower is better; medians are over 1085 runs for (a), 872 for (b).

Here we have actually acquired the full test set. This lets us show that both \( R_{\text{LURE}} \) and \( R_{\text{id}} \) converge to the empirical test loss on the entire test set. However, typically we cannot do this which makes the difference in variance between \( R_{\text{id}} \) and \( R_{\text{LURE}} \) at lower acquisition numbers crucial.

5.2. Surrogate Choice Case Study: Image Classification

We now investigate the impact of the different surrogate choices. For this, we move to more complex image classification tasks and additionally restrict the number of training points to only 250. This makes it harder to predict the true loss. Therefore, the strategies discussed in §3.4 are especially important to maximize sample-efficiency.

We evaluate two model types for this examination. First, a Radial Bayesian Neural Network (Radial BNN) (Farquhar et al., 2020) on the MNIST dataset (LeCun et al., 1998) in Fig. 4 (a). Radial BNNs are a recent approach for variational inference in BNNs (Blundell et al., 2015) and we use them because of their well-calibrated uncertainties.

We also evaluate a ResNet-18 (He et al., 2016) trained on Fashion-MNIST (Xiao et al., 2017) in Fig. 4 (b) to investigate active testing with conventional neural network architectures. In these figures, we show the median squared error of the different surrogate strategies on a logarithmic scale to highlight differences between the approaches. While not shown, note that all approaches do still obtain unbiased estimates. We again use Eq. (12) to estimate the cross-entropy loss of the models.

Predictive Entropy. We first consider the most naive of the approaches mentioned in §3.4: using the unchanged original model as the surrogate, which leads to acquisitions based on model predictive entropy. For the Radial BNN, this approach already yields improvements over i.i.d. acquisition in Fig. 4 (a). The same can not be said for the ResNet in Fig. 4 (b), for which predictive entropy actually performs worse than i.i.d. acquisition. Presumably, this is the case because the standard neural network struggles to model epistemic uncertainty. Now, we progress to more complex surrogates, improving performance over the naive approach.

Retraining. BNN surrogate is a surrogate with identical setup as the original model that is re-trained on the total observed data, \( D_{\text{train}} \cup D_{\text{test}}^{\text{observed}} \), 12 times with increasingly large gaps. This leads to improved performance over the naive model predictive entropy, especially as more data is acquired. Similarly, the ResNet surrogate shows much-improved performance over predictive entropy when regularly re-trained, now outperforming i.i.d. acquisition.

Different Model. As discussed in §3.4, it may be beneficial to choose the surrogate from a different model family to promote diversity in its predictions. We use a random forest as a surrogate for both Fig. 4 (a) and (b). For the Radial BNN on MNIST, the random forest, while better than i.i.d. acquisition, does not improve over the model predictive entropy. However, for the ResNet on Fashion-MNIST, we find that the random forest surrogate outperforms everything, despite being a cheaper surrogate. This demonstrates that for a surrogate to be successful, it does not necessarily need to be more accurate—although the difference in accuracy is small with so few data. Instead, the surrogate can be also be successful by being different from the original model, i.e. having structural biases that lead to it making different predictions and therefore discovering mistakes of the original model, with any new mistakes made less important. Further, if compute is limited, the random forest is attractive because retraining it is much faster.

Ensembling Diversity. §3.4 discussed two ways retraining may help: new data improves the surrogate’s predictive model and repeated training promotes diversity through an implicit ensemble. In Fig. 4 (b), we introduce the ResNet train ensemble—a deep ensemble of ResNets trained once on \( D_{\text{train}} \). This surrogate allows us to isolate the effect of predictive diversity since it is not exposed to any test data through retraining. We output mean predictions of the ensemble, and find that the deep ensemble can, a little unexpectedly, outperform the ResNet surrogate without accessing the extra data. This is likely because of better calibrated uncertainties and the increased model capacity.

In summary, we have shown that active testing reduces the number of labeled examples required to get a reliable estimate of the test loss for a Radial BNN on MNIST and
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ResNet-18 on FashionMNIST in a challenging setting, if appropriate surrogates are chosen.

5.3. Large-Scale Image Classification

We now additionally apply active testing to a ResNet-18 trained on CIFAR-10 (Krizhevsky et al., 2009) and a WideResNet (Zagoruyko & Komodakis, 2016) trained on CIFAR-100. As the complexity of the datasets increases, it becomes harder to estimate the loss, and hence, it is crucial to show that active testing scales to these scenarios. We use conventional training set sizes of 50,000 data points.

In the previous section, we have seen surrogates based on deep ensembles perform well, even if they are only trained once and not exposed to any acquired test labels. For the following experiments, we therefore use these ensembles as surrogates. This is even more justified in the common case where there is much more training data than test data; the extra information in the test labels will typically help less.

In Fig. 5, we further visualize how ensembles increase the quality of the approximated loss in this setting. The original model (b) makes overconfident false predictions with high losses which are rarely detected (box). But the ensemble avoids the majority of these mistakes (c, box) which contribute most to the weighted loss estimator Eq. (3).

In all cases, the active testing estimator has lower median squared error than the baseline, see Fig. 6 (a)—again note the log-scale. We further show in Fig. 6 (b) that using active testing is much more sample-efficient than i.i.d. sampling by calculating the ‘relative labeling cost’; the proportion of actively chosen points needed to get the same performance as naive uniform sampling. E.g., a cost of 0.25 means we need only 1/4 of actively chosen labels to get equivalently precise test loss. Thus, for the less complex datasets, we see efficiency gains are in the region of a factor of four, while for CIFAR-100 they are closer to a factor of two. We also show that there are similar gains in sample-efficiency when estimating accuracy—‘CIFAR-10 Accuracy’ in Fig. 6 (b).

5.4. Diversity and Fidelity in Ensemble Surrogates

We now perform an ablation to study the relative effects of surrogate fidelity and diversity on active testing performance. For this, we evaluate a ResNet-18 trained on CIFAR-10 using different ResNet ensembles as surrogates. Starting with a base surrogate of a single ResNet-18, we increase the size of the ensemble (mainly increasing diversity) as well as the capacity of the layers (increasing fidelity). Given the success of the ‘Train Ensemble’ in §5.2, we train surrogates only once on $D_{\text{train}}$, rather than retraining as data is acquired.

As Fig. 7 shows, both fidelity and diversity contribute to active testing performance: the best performance is obtained for the most diverse and complex surrogate, justifying our claims in §3.4. We see that increasing fidelity and diversity both individually help performance, with the effect of the latter seeming to be most pronounced (e.g. an ensemble of 5 ResNet-18s outperforms a single ResNet-50).

5.5. Optimal Proposals and Unbiasedness

Fig. 8 (a) confirms our theoretical assumptions by showing that sampling proportional to the true loss, i.e. cheating by asking an oracle for the true outcomes beforehand, does indeed yield exact, single-sample estimates of the loss if
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Figure 7. Both diversity and fidelity of the surrogate contribute to sample-efficient active testing. However, the effect of increasing diversity seems larger than that of increased fidelity. We vary the layers (fidelity) and ensemble size (diversity) of the surrogate for active evaluation of a ResNet-18 trained on CIFAR-10. Experiments are repeated for 1000 randomly drawn test sets and we report average values over acquisition steps 100–200.

5.6. Active Testing vs. Active Learning

As mentioned in §3.4, we expect there to be differences in acquisition function requirements for active learning and active testing. For example, mutual information is a popular acquisition function in active learning (Houlsby et al., 2011), but our derivations for classification lead to acquisition strategies based on predictive entropy. Can mutual information also be used for active testing? In Fig. 8 (b) we see that even the simple approach of using the original model as a surrogate and a predictive entropy acquisition outperforms mutual information. Acquiring with mutual information helps active learning because it focuses on uncertainty that can be reduced by more information rather than irreducible noise. While this focus helps learning, it is unhelpful for evaluation where all uncertainty is relevant. This is just one way active testing needs special examination and cannot just re-use results from active learning.

5.7. Practical Advice

Empirically, we find that deep learning ensemble surrogates appear to robustly achieve sample-efficient active testing when using our acquisition strategies. Increases in surrogate fidelity further seem to benefit sample-efficiency.

Active testing generally assumes that acquisitions of labels for samples are expensive, hence we recommend retraining the surrogate whenever new data becomes available. However, if the cost of this is noticeable relative to that of labeling, our results indicate that not retraining the surrogates is an option, especially when the number of acquired test labels is small compared to the training data.

In general, we do not recommend the naive strategy that relies entirely on the original model and does not introduce a dedicated surrogate model. As §5.2 has shown, this method can fail to achieve sample-efficient active testing if the original model does not have trustworthy uncertainties. This strategy should remain a last resort and used only when there is significant reason to trust the original model’s uncertainties; we find the diversity provided by a surrogate is critical, even if that surrogate is itself simple.

6. Conclusions

We have introduced the concept of active testing and given principled derivations for acquisition functions suitable for model evaluation. Active testing allows much more precise estimates of test loss and accuracy using fewer data labels.

While our work provides an exciting starting point for active testing, we believe that the underlying idea of sample-efficient evaluation leaves significant scope for further development and alternative approaches. We therefore eagerly anticipate what might be achieved with future work.

Acknowledgements

We acknowledge funding from the New College Yeotown Scholarship (JK) and Oxford CDT in Cyber Security (SF).
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A. Additional Experiments

A.1. Synthetic Data

Figure A.1 shows experiments on additional synthetic data together with the experiments familiar from Fig. 3 of the main paper. We show two additional regression settings: a GP on sinusoidal data with non-uniform densities in $x$ and a GP on the quadratic data already familiar from Fig. 3 (b). Active testing yields gains in sample-efficiency for both of these additional settings. We give details for all synthetic experiments in Appendix C.2.

A.2. Radial BNN on MNIST

We also investigate active testing of a Radial BNN on MNIST in a large data regime with 50,000 training points. As acquisition strategy, we here simply use the predictive entropy of the Radial BNN, which we observe to be well-calibrated in this simple setting. Consequently, we see large gains in sample-efficiency of active testing over i.i.d. acquisition for this setting as shown in Fig. A.2. We discuss experimental details for this plot in Appendix C.8.

A.3. Uncertainties and Statistical Significance

In Figs. A.3 to A.5, we show a variation of Figs. 4, 6 (a), and 8 (b) wherein we plot mean log squared differences instead of median squared differences. All conclusions from the main body of the paper continue to hold for the mean-based visualization. Additionally, we quantify uncertainties on the mean values via the standard errors of the log squared differences.

We also investigate the statistical significance of the results reported in the paper, computing Wilcoxon signed-rank test statistics to examine if the best active testing strategy has lower population mean rank than all other shown methods. More precisely, when comparing two methods at a fixed acquisition step, we obtain a pair of samples of squared differences for each run, and we test against the alternative hypothesis that the best performing method has lower squared error. We compare methods at the last displayed acquisition step. The results of the test show that we can always reject the null hypothesis at $5 \times 10^{-3}$ confidence level. We give the full results of the Wilcoxon signed-rank tests in Table 1.

B. Details on Active Testing

B.1. Further Details on Clipping

As mentioned briefly in the main paper, we are clipping the predicted $q(i_m)$ to avoid overly small acquisition values. We do this because $R_{LURE}$ is only unbiased if we have non-zero acquisition probability on all points remaining (Farquhar et al., 2021). In practice, we bound the value of the acquisition function from below at $\alpha$ times the acquisition probability assigned by a uniform acquisition strategy, where $\alpha = 0.2$.

B.2. Computational Complexity

Two components of active testing contribute significantly to computational complexity: Evaluating the acquisition function on the remaining samples of the test pool and retraining the surrogate on all observed samples.

**Acquisition Function Evaluation.** At each active testing iteration, we require the evaluation of the acquisition function $q$ on all remaining samples in the test pool $D_{\text{test}}$. At first iteration, $N$ samples remain in the test pool, contributing $O(N)$ to the computational complexity. At each subsequent iteration $m$, $O(N - m)$ additional evaluations are required. For a total

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2Reminder: We calculate the squared difference between the true test loss on the full test set (known only to an oracle) and the estimator at each acquisition step.
### Active Testing: Sample-Efficient Model Evaluation

| Model / Data | GP / GP / GP Prior | GP / GP / Quadratic | GP / GP / Sinusoidal | Linear / GP / Quadratic | RF / RF / Two Moons |
|-------------|--------------------|---------------------|----------------------|------------------------|---------------------|

| Number of Acquired Test Points | 1  | 20  | 40  | 1  | 20  | 40  |
|-------------------------------|----|-----|-----|----|-----|-----|
| Difference to Full Test Loss  |    |     |     |    |     |     |

**Figure A.1.** Active testing on synthetic data. Columns (1, 4, 5) are repeated from Fig. 3 of the main paper, while (2–3) are exclusive to the appendix. Each column shows a different combination of model/surrogate/data. The first row shows model predictions, as well as the points used for training and testing for a single draw from the random data generation. The second row displays the mean difference of the estimators to the true loss on the full test set (known only to an oracle).

| Acquired Points | 1 | 500 | 1000 |
|-----------------|---|-----|------|
| Difference to Full Test Loss | $\times 10^{-2}$ |     |      |

| Acquired Points | 1 | 500 | 1000 |
|-----------------|---|-----|------|
| Median Squared Error | $10^{-3}$ | $10^{-4}$ | $10^{-5}$ |

| Acquired Points | 1 | 100 | 200 |
|-----------------|---|-----|-----|
| Relative Labeling Cost | 0 | 0.5 | 1 |

**Figure A.2.** Active testing for a Radial BNN on MNIST using model predictive entropy to estimate test cross-entropy loss. (a) Active testing gives unbiased loss estimators with (b) much lower median squared error. (c) We calculate the relative labelling cost: the sample-efficiency factor of i.i.d. acquisition to active testing at any number of acquired points. Lower is better and values less than 1 are gains in sample-efficiency. We plot medians and quantiles (0.1, 0.9) and average over 992 runs.

Surrogate Retraining. In our experiments in §5.2, we demonstrate successful active testing when retraining the surrogate every $K$ steps or training the surrogate only once on $D_{\text{train}}$. However, in active testing practice, label cost may be significantly larger than the cost of retraining. Therefore, we here assume the worst case $K = M$, i.e. retraining the surrogate after each acquisition. This gives maximum sample-efficiency because additional information from newly acquired test labels is directly used to improve surrogate predictions. At first iteration, only $D_{\text{train}}$ is observed and hence retraining costs will be $O(|D_{\text{train}}|)$. As testing progresses, $m$ samples of the test set become available such that retraining costs grow to $O(|D_{\text{train}}| + m)$ per iteration. For a total of $M$ acquisitions, retraining costs therefore scale as $O(M|D_{\text{train}}| + M^2)$. Therefore, we can bound the total computational complexity of active testing as $O(M|D_{\text{train}}| + M^2 + MN)$, which can be simplified to $O(M|D_{\text{train}}| + MN)$ as $M \leq N$ always.

### C. Details on Experiments

#### C.1. Hardware

For the neural network architectures, we use PyTorch (Paszke et al., 2019). We use a mix of NVIDIA RTX 2080, Titan RTX, and K80 GPUs to run the experiments. No experiment requires more than one GPU in parallel. Experiments that do not require GPUs, such as the synthetic data experiments, can be run on CPUs only on conventional hardware.
Active Testing: Sample-Efficient Model Evaluation

Table 1. Wilcoxon signed-rank tests for experiments from the main paper, comparing the squared differences of the best method against all other shown approaches. The alternative hypothesis is that the ‘best method’ has lower squared error than the ‘other method’.

| Figure | Dataset          | Best Method               | Other Method                  | Acq. Step | p-Value         |
|--------|------------------|---------------------------|-------------------------------|-----------|-----------------|
| 4 a    | MNIST            | BNN Surrogate             | I.I.D. Acquisition           | 1000      | $5.438 \times 10^{-61}$ |
|        | MNIST            | BNN Surrogate             | Random Forrest Surrogate      | 1000      | $7.069 \times 10^{-19}$ |
|        | MNIST            | BNN Surrogate             | Original Model                | 1000      | $9.524 \times 10^{-20}$ |
| 4 b    | Fashion-MNIST    | Random Forrest Surrogate  | Original Model                | 1000      | $6.586 \times 10^{-125}$ |
|        | Fashion-MNIST    | Random Forrest Surrogate  | I.I.D. Acquisition            | 1000      | $4.176 \times 10^{-31}$  |
|        | Fashion-MNIST    | Random Forrest Surrogate  | ResNet Surrogate              | 1000      | $4.249 \times 10^{-17}$  |
|        | Fashion-MNIST    | Random Forrest Surrogate  | ResNet Train Ensemble         | 1000      | $4.254 \times 10^{-10}$  |
| 6 a    | CIFAR-100        | ResNet Train Ensemble     | I.I.D. Acquisition            | 500       | $3.010 \times 10^{-11}$  |
|        | CIFAR-10         | ResNet Train Ensemble     | I.I.D. Acquisition            | 500       | $3.988 \times 10^{-76}$   |
|        | Fashion-MNIST    | ResNet Train Ensemble     | I.I.D. Acquisition            | 500       | $2.457 \times 10^{-105}$  |
| 7      | Fashion-MNIST    | Predictive Entropy        | I.I.D. Acquisition            | 400       | $2.801 \times 10^{-6}$    |
|        | Fashion-MNIST    | Predictive Entropy        | Mutual Information            | 400       | $8.779 \times 10^{-4}$    |

C.2. Figures 1 to 3: Synthetic Data

We now give details for Fig. 3 of the main paper, shown again in Fig. A.1 (columns 1, 4, 5), as well as the additional experiments (columns 3 and 4). Figures 1 and 2 use the setup of Fig. A.1 (column 1).

Regression. For the Gaussian process data (column 1), we sample $N = 50$ points from a Gaussian process with Matern-Kernel $\nu = 3/2$ and $l = 1$, using the implementation of Pedregosa et al. (2011). For each of the experiments, we sample a different set of points from the Gaussian process prior. The quadratic data (columns 2, 4) are drawn from $f(x) = y^2$. The sinusoidal data (column 3) are drawn from $f(x) = \sin(10x) + x^3$, where the density of the samples in $x$ is non-uniform.

5 points are randomly assigned to the training set, 45 are used for testing. The test-train assignments are randomly redrawn between experiments. For each experiment, we actively evaluate the data with all acquisition functions. We perform a series of 5000 independent experiments. All regression experiments use a Gaussian process surrogate that is retrained after each acquisition on all observed data and has Matern-Kernel $\nu = 3/2$ and $l = 1$.

Two Moons Classification. For the two moons dataset (column 5), we randomly sample $N = 500$ points with noise level of 0.1 for each experiment, using the implementation of Pedregosa et al. (2011). 50 points are randomly assigned to the training set, 450 are used for testing. We perform a series of 2500 independent experiments. We use default parameters and implementation of Pedregosa et al. (2011) for the random forest. The surrogate model uses an identical random forest that is retrained after each acquisition on all observed data.

C.3. Figure 4: Radial BNN/ResNet-18 on MNIST/Fashion-MNIST

Data. For each experiment, we sample 250 training and 5000 test points randomly from the combined training and test set of the original datasets. We standardize the dataset using per-channel mean and standard deviation values over all pixels of the training set. We actively acquire 1000 samples from the test set and compute the ‘full test loss’ on all 5000 test points. We perform stratified sampling for both the train/test as well as the train/val splits. We retrain the surrogates after acquiring (0, 5, 10, 20, 30, 40, 100, 250, 400, 550, 700, 850, 1000) test points.

Radial BNN on MNIST. We use the code obtained from Farquhar et al. (2021) to implement the Radial BNNs. We use the following hyperparameters, which are default values taken from Farquhar et al. (2021): we use a learning rate of $1 \times 10^{-4}$ and weight decay of $1 \times 10^{-4}$ with the ADAM optimizer (Kingma & Ba, 2014), batch size of 64, 8 variational samples during training for the BNN, 100 variational samples during testing, and convolutions with 16 channels. We train for a maximum of 500 epochs with early stopping patience of 5 and use validation sets of size 50. We have not tuned these hyperparameters.

ResNet-18 on Fashion-MNIST. For Resnet-18, we use the default hyperparameter values introduced by DeVries & Taylor (2017): we use a learning rate of 0.1, weight decay of $5 \times 10^{-4}$, and momentum of 0.9 with an SGD optimizer, and batch
size of 128. We use a cosine annealing schedule for the learning rate as provided by PyTorch. We train for a maximum of 160 epochs with early stopping patience of 20 and use validation sets of size 50. We have not tuned these hyperparameters.

**Random Forest Surrogate.** We use random forests with 100 estimators, split criterion ‘entropy’, and maximum number of features considered at each split proportional to the square root, otherwise using the default parameters and implementation of Pedregosa et al. (2011). Hyperparameters were set with a single grid-search cross-validation on one particular training set.

**Training Convergence: Radial BNN on MNIST.** Training of the BNN takes about 1 to 2 minutes and the early stop patience usually terminates training after around 50 to 100 epochs. A single experiment run for the Radial BNN, requiring the training of the original model and retraining of all shown surrogates, takes about 30 minutes. The validation accuracy on the initial 250 points is at about 80 to 90 percent and grows to about 90 to 98 percent after observing a total of 1250 points. We perform a total of 1085 runs.

**Training Convergence: ResNet-18 on Fashion-MNIST.** Training of the ResNet takes about 10 to 40 seconds and the early stop patience sets in around 30 to 80 epochs. A single run for the ResNet, requiring the training of the original model and retraining of all shown surrogates, takes about 10 minutes. The training validation accuracy on the initial 250 points is at about 68 to 78 percent and grows to about 80 to 86 percent after observing a total of 1250 points. We perform a total of 872 runs.
Active Testing: Sample-Efficient Model Evaluation

Figure A.4. Figure 6 (a) from the main paper but now showing the mean of the log squared difference instead of the median. Additionally, shading indicates the standard error of the log squared difference. Averages over 1000 random test set draws. See text and main paper for details.

Figure A.5. Figure 8 (b) from the main paper but now showing the mean of the log squared difference instead of the median. Additionally, shading indicates the standard error of the log squared difference. Averages over 692 runs. See text and main paper for details.

C.4. Figure 5: ResNet-18 on CIFAR-100

The setup for Fig. 5 is a ResNet-18 on CIFAR-100 identical to the experiments from Fig. 6 described in the following. The model converges to 72 to 76 percent accuracy in about 12 minutes and we perform 692 runs.

C.5. Figure 6: ResNet-18/WideResNet on Fashion-MNIST, CIFAR-10/Cifar-100

Data. We now respect the original train and test indices of the dataset. We train a model on the training set and then, for each experiment, perform active testing on a subset of 1000 randomly sampled points from the original test set of size 10,000. We standardize the dataset using per-channel mean and standard deviation values over all pixels of the training set. For CIFAR-10 and CIFAR-100, we apply random crops and horizontal flips to the training data in each epoch. Given the larger training data, we now use validation sets of size 2560. We re-sample test sets for the next experiment, but keep training sets and models constant. We perform stratified sampling for both the train/test as well as the train/val splits. This, we repeat a total of 1000 times.

ResNet-18. Unless otherwise mentioned we use identical hyperparameters as for Fig. 4. On all datasets, we train for a maximum of 30 epochs with patience of 5. Again, we do not systematically tune hyperparameters and only make
adjustments to accommodate the increased data size compared to Fig. 4. The model converges to 93 to 94 percent accuracy on Fashion-MNIST in about 7 minutes and 92 to 93 percent accuracy on CIFAR-10 in about 12 minutes.

**WideResNet.** We use a WideResNet of depth 40 and the setup introduced by DeVries & Taylor (2017): we train for 200 epochs, use a learning rate of 0.1, weight decay of $5 \times 10^{-4}$, and momentum of 0.9 with an SGD optimizer, and batch size of 128. We also use the scheduler of DeVries & Taylor (2017) and decrease the learning rate by a factor of $\gamma = 0.2$ at epochs 60, 120, and 160. The model converges to 78 to 80 percent accuracy on CIFAR-100 in about 240 minutes.

**Ensembles.** For the deep ensemble of Resnet-18s, we use 10 models for Fashion-MNIST, 5 for CIFAR-10, and 15 for CIFAR-100. For the deep ensemble of WideResnets on CIFAR-100, we use a set of 10 models. The models for the ensembles are identical to the main models, i.e. use the same hyperparameters, optimizers, and training setup, and only differ in terms of the optima reached from stochastic model initialization and optimization.

Increasing the size of the ensemble did sometimes yield improved results. Following initial experiments, we increased the size of the ensemble for Fashion-MNIST from 5 to 10. However, using ensemble size of 15 on CIFAR-10 did not improve the results noticeably (nor worsen them), so we display the smaller, and computationally cheaper ensemble in the main body.

**C.6. Figure 7**

Figure 7 uses the same setup as Fig. 6 for CIFAR-10 with main ResNet-18 model and ‘train ensemble’-style surrogates.

**C.7. Figure 8**

For the Radial BNN, Fig. 8 uses identical experimental setup as Fig. 4, except that the model is trained for a maximum of 30 epochs (patience 5) and we use validation sets of size 1280, to account for the increase in data. For the Fashion-MNIST data, we concatenate the original train and test datasets, from which we then sample 50,000 points without replacement for the training dataset and 10,000 for the test dataset. We acquire a total of 1000 points from the test dataset but compute the ‘full test set loss’ on all 10,000 points. Splits are stratified by class labels. We redraw train and test splits, and retrain models between runs. For each experiment, the model reaches about 88 to 92 percent validation accuracy in about 8 minutes. We perform a total of 962 runs.

**C.8. Figure A2: Radial BNN on MNIST.**

For the Radial BNN, Fig. A.2 uses identical experimental setup as Fig. 4 (a), except that the model is trained for a maximum of 50 epochs (patience 5) and we use validation sets of size 1280 to account for the increase in data. For the MNIST data, the setup is identical to Fig. 8. The model reaches about 98 percent validation accuracy in about 7 to 10 minutes. We perform a total of 992 runs.

**D. Comparison to Active Risk Estimation by Sawade et al.**

We here provide a brief introduction to ‘Active Risk Estimation’ (ARE) by Sawade et al. (2010) as well as an empirical comparison of their approach to ours. Similar to us, Sawade et al. (2010) actively acquire labels from a test pool of unlabeled samples, aiming to obtain a sample-efficient estimate of the empirical test risk. However, unlike us, they do not fully accommodate the pool-based setting. Additionally, Sawade et al. (2010) rely only on the original model to approximate outcomes $y \mid x$, while we have shown that appropriate surrogate models can be crucial for sample-efficient active testing. Moreover, as we show below, active testing outperforms ARE in practice.

**D.1. Background**

Sawade et al. (2010) derive an ‘optimal acquisition function’

$$q^*(x) \propto p(x) \sqrt{\int \mathcal{L}(f_\theta(x), y) - R_i^2 \ p(y \mid x) \ dy},$$

(15)

where $R = \mathbb{E} [\mathcal{L}(f(x), y)]$ is the true model risk. For the pool-based setting, they obtain an equivalent ‘optimal acquisition function’ by setting $p(x_{in}) = \frac{1}{M}$ and approximating $R$ with the empirical test risk $R_{iid}$ over the entire test pool. As $R_{iid}$ is still unknown, Sawade et al. (2010) approximate $R_{iid}$ using the original model’s mean predictions $f_\theta(x)$ to approximate the
Figure D.1. Comparison of Active Testing to Active Risk Estimation (ARE) by Sawade et al. (2010). (a) While active testing can yield single-sample zero-variance optimal estimates, ARE cannot because it does not fully accommodate the pool-based setting. (b) Naive extensions of ARE to sampling without replacement are unsuccessful. (c) In practice, ARE yields lower performance than active testing. (d) As test set grows, the gap between ARE and active testing will get smaller as sampling with replacement matters less. Dashed grey line demarcates number of samples in the test pool. Solid lines show means, dashed lines standard deviations over 7000 (a–c) / 2000 (d) runs.

true outcomes, giving

\[
\hat{R}_{\text{i.i.d.},\theta} = \frac{1}{M} \sum_{x \in \mathcal{D}_{\text{test}}} \int \mathcal{L}(f_\theta(x), y)p(y|x; \theta) \, dy
\]

\[
q^*(x) \propto \sqrt{\int \left[ \mathcal{L}(f_\theta(x), y) - \hat{R}_{\text{i.i.d.},\theta} \right]^2 p(y | x; \theta) \, dy}.
\]

They do not consider the concept of a surrogate model.

Plugging mean squared error loss and Gaussian likelihoods into (17), they derive the acquisition function

\[
q(x) \propto \sqrt{3\sigma_x^4 - 2\hat{R}_{\text{i.i.d.},\theta}\sigma_x^2 + \hat{R}_{\text{i.i.d.},\theta}^2},
\]

where \(\sigma_x^2\) is the total predictive variance (aleatoric and epistemic uncertainty) of the original model’s prediction at \(x\).

For risk estimation, ARE relies on a standard importance sampling estimator

\[
\hat{R}_{\text{IS}} = \frac{1}{M} \sum_{m=1}^{M} \frac{1}{q(x_{im})} \mathcal{L}(f_\theta(x_{im}, y_{im})) \]

where the uniform \(p(x_{im})\) cancels from the weights. Unlike \(\hat{R}_{\text{LURE}}\), \(\hat{R}_{\text{IS}}\) requires sampling with replacement to obtain unbiased estimates. In other words, ARE does not remove samples from the test pool after querying them, and often, test points will get sampled repeatedly.
D.2. Empirical Comparison.

We compare both theoretically optimal behavior as well as observed practical performance of our active testing and ARE. For this, we take the familiar setup from Fig. A.1 (column 1).

Optimal Behavior. We have seen that active testing can ideally lead to single-sample, zero variance estimates of the test loss (cf. Fig. 8 (a)). What is the optimal behavior ARE can obtain? To test this, we apply (15) with the oracle empirical test risk $\hat{R}^\text{i.i.d.}$ and the true $y|x$ (which is a $\delta$-distribution since we generate data without noise). This constitutes the best case scenario for ARE performance.

As Fig. D.1 (a) shows, ‘optimal ARE’ can improve over i.i.d. acquisition but does not show the same desirable single-sample optimal behavior as active testing. Note that ARE extends beyond the test set size of 45 because it does not naturally converge due to sampling with replacement. In Fig. D.1 (b) we confirm that naive extensions of ARE to sampling without replacement are not successful: (i) Simply using ARE but sampling without replacement does not work; (ii) When additionally using $\hat{R}^\text{i.i.d.}$ instead of $\hat{R}^\text{IS}$, we converge to the empirical test risk but observe a bias and increased variance over i.i.d. acquisition at earlier acquisition steps.

Performance in Practice. We now investigate behavior of ARE in practice—where the oracle risk is not available and we rely on (17) instead. Figure D.1 (c) shows that while ARE can increase sample-efficiency over i.i.d. acquisition in practice, it is clearly outperformed by active testing. For Fig. D.1 (d), we increase the size of the test set from 45 to 295. We suspect that further increases in test set size will shrink the gap between ARE and active testing without surrogates, because sampling with replacement should become less important. However, still, active testing clearly outperforms ARE: active testing also varies substantially in the acquisition strategy it uses (in particular allowing the use of surrogates), with these result suggesting its approach is clearly preferable.

Redefining Acquisitions Steps. Sampling with replacement is a sub-optimal strategy for methods applied in pool-based...
settings. As mentioned above, sampling with replacement in ARE leads to the same samples being acquired multiple times. For maximum fairness, we now only increase the ‘acquisition step’ counter by one if the sampling with replacement process leads to an acquisition that has not been previously made, i.e. if the acquisition is novel. This is somewhat justified in practice because we assume that acquiring novel labels is much more expensive than acquisition function evaluations.

However, find that ARE leads to a significant increase in queries compared to active testing\(^3\) and still performs far worse even by this beneficial metric. Namely, we display the results with ‘rescaled x-axis’ in Fig. D.2. While the performance of ARE appears slightly improved, our overall conclusions are unaffected.

\(^3\)For Fig. D.1 (c), ARE takes (9.8 ± 3.1) as many queries as there are samples in the test pool. This number will increase for larger test pools and shows that sampling with replacement is not a desirable strategy for pool-based active model evaluation.