
Sequential Covariate Shift Detection Using Classifier Two-Sample Tests

Sooyong Jang¹ Sangdon Park^{1,2} Insup Lee¹ Osbert Bastani¹

Abstract

A standard assumption in supervised learning is that the training data and test data are from the same distribution. However, this assumption often fails to hold in practice, which can cause the learned model to perform poorly. We consider the problem of detecting *covariate shift*, where the covariate distribution shifts but the conditional distribution of labels given covariates remains the same. This problem can naturally be solved using a two-sample test—*i.e.*, test whether the current test distribution of covariates equals the training distribution of covariates. Our algorithm builds on *classifier tests*, which train a discriminator to distinguish train and test covariates, and then use the accuracy of this discriminator as a test statistic. A key challenge is that classifier tests assume given a fixed set of test covariates. In practice, test covariates often arrive sequentially over time—*e.g.*, a self-driving car observes a stream of images while driving. Furthermore, covariate shift can occur multiple times—*i.e.*, shift and then shift back later or gradually shift over time. To address these challenges, our algorithm trains the discriminator online. Additionally, it evaluates test accuracy using each new covariate before taking a gradient step; this strategy avoids constructing a held-out test set, which can improve sample efficiency. We prove that this optimization preserves the correctness—*i.e.*, our algorithm achieves a desired bound on the false positive rate. In our experiments, we show that our algorithm efficiently detects covariate shifts on multiple datasets—ImageNet, IWild-Cam, and Py150.

1. Introduction

A key challenge facing deep neural networks is their sensitivity to changes in the data distribution. In particular, supervised learning traditionally assumes that the training and test data are from the same distribution (Vapnik, 1998), but this assumption often fails in practice. For example, an autonomous car using perception to identify obstacles needs to be robust to shifts such as changes in the weather and lighting conditions. We focus on *covariate shift* (Shimodaira, 2000), where there is a shift in the covariate distribution $p(x)$, and the conditional label distribution $p(y | x)$ remains unchanged. Covariate shift can reduce model performance (Sugiyama & Müller, 2005), invalidate uncertainty estimates (Ovadia et al., 2019; Park et al., 2020), and affect model selection (Sugiyama et al., 2007).

One strategy is to devise an algorithm to detect covariate shift; if detected, the algorithm can alert the user that predictions may be unreliable. Covariate shift detection can be formulated as two-sample hypothesis test (Gretton et al., 2012a; Rabanser et al., 2018; Liu et al., 2020), where the goal is to determine whether two sets of examples are from the same distribution. To test for covariate shift, we choose the first sample to be the data used to train the model and the second sample to be recent test data given as input to the model. Then, the detector returns “covariate shift” if the hypothesis test indicates that the two samples are from different distributions and “no shift” otherwise.

We propose a detection algorithm based on classifier tests (Lopez-Paz & Oquab, 2017; Cheng & Cloninger, 2019; Kim et al., 2021), which use the accuracy of a classifier trained to distinguish the two samples as the test statistic. In particular, if the two samples are from the same distribution, then the accuracy should be $1/2$; otherwise, it should be $> 1/2$. Since the test statistic follows a binomial distribution, we use the Clopper-Pearson interval (Clopper & Pearson, 1934) (an exact confidence interval for the unknown success probability of the Binomial distribution) to derive the cutoff. In contrast, prior work relies on asymptotics to derive the cutoff, which results in approximations.

A key challenge is that the test examples are typically obtained over time—*e.g.*, an autonomous robot continuously perceives its environment, and we want to detect if its distribution of observations shifts at any time. There are two

¹PRECISE Center, University of Pennsylvania, USA.

²School of Cybersecurity and Privacy, Georgia Institute of Technology, USA. Correspondence to: Sooyong Jang <sooyong@seas.upenn.edu>.

key challenges to leveraging classifier tests in this setting. First, they rely on training a classifier to distinguish training and test examples; doing so on every step would be computationally intractable. Second, they rely on a held-out test set to estimate the test statistic, but constructing such a set online would reduce sample efficiency.

Rather than train a classifier at each step, our algorithm trains a model online using stochastic gradient descent. Then, rather than construct a held-out test set, our algorithm evaluates the accuracy of the model online using each example before taking a gradient step on that example. We prove that this strategy results in an unbiased estimate of the model accuracy; thus, the finite-sample guarantees on the false positive rate provided by the sequential test continue to hold. In addition, we prove bounds on the false negative rate under mild conditions on the classifier (i.e., it achieves nontrivial accuracy distinguishing the two distributions).

We evaluate our approach on both synthetic and natural shifts on ImageNet (Russakovsky et al., 2015), and natural shifts on two datasets from the WILDS datasets (Koh et al., 2021). We demonstrate that our approach achieves better sample efficiency than baseline algorithms; furthermore, it satisfies the desired false positive rate. Thus, our algorithm is an effective strategy for sequential covariate shift detection.

Contributions. We formulate (sequential) covariate shift detection as a two-sample test, and propose a novel algorithm to solve this problem (Section 3). Then, we prove finite sample bounds on false positive rate and false negative rate achieved by our algorithm (Section 4). Finally, we empirically demonstrate that our algorithm effectively detects shifts on ImageNet, IWildCam, and Py150 (Section 5 and Appendix C).

Sequential detection vs. sequential tests. While we consider the sequential setting, we deliberately choose not use a sequential hypothesis test, since the covariate shift may occur after a delay or gradually over time. A sequential test only applies if *all* of the test data is shifted. Furthermore, since we are not using sequential tests, the false positive rate bound only holds per-step, not uniformly across all steps. This is necessary: we cannot guarantee that we detect a covariate shift occurring at a later point in time if we constrain the false positive to be bounded uniformly across all steps. In our experiments, we show that the rate of false alarms remains manageable while enabling our algorithm to detect covariate shift in a number of interesting scenarios.

2. Related Work

Covariate shift. There has been work on training models in the presence of covariate shift. In particular, in the unsupervised domain adaptation setting (Ben-David et al., 2007;

Bickel et al., 2007; Ganin et al., 2016), the algorithm has access to labeled examples from the source domain but only unlabeled examples from the target domain, and the goal is to train a model that achieves good performance on the target domain. One strategy is to use importance weighting to upweight source examples that are more similar to target examples (Bickel et al., 2007). Another strategy is to first learn an invariant representation (Ganin et al., 2016), which is an embedding space where the source and target examples are similar, and then train a model on this embedding space using the source examples. If we detect covariate shift, one solution is to retrain the model using these techniques.

Two-sample tests. We focus on *classifier two-sample tests* (C2ST). In this approach, the idea is to train a binary classifier to distinguish source and target samples, compute a real-valued score based on this classifier as the test statistic, and then use a univariate two-sample test to determine the cutoff for rejecting the null hypothesis (Friedman, 2004). A natural test statistic is the classifier’s accuracy on a held-out test set (Kim et al., 2021; Lopez-Paz & Oquab, 2017), or the differences in the classifier’s logits (Cheng & Cloninger, 2019); we use the former. One way to compute the cutoff is to use the asymptotic distribution of the test statistic (Lopez-Paz & Oquab, 2017). Nonparametric tests such as permutation tests can also be used (Kim et al., 2021).

Another kind of two-sample test is a *kernel two-sample test*. Here, the idea is to use the maximum mean discrepancy (MMD) between the two samples according to a given kernel embedding as the test statistic (Gretton et al., 2012a; Chwialkowski et al., 2015; Jitkrittum et al., 2016). The key design decision is the choice of kernel. One strategy is to use a nonparametric kernel such as Gaussian radial basis functions (Gretton et al., 2012a); alternatively, the kernel can also be optimized to minimize the false negative rate of the resulting test (Gretton et al., 2012b). Recent work has shown how to first learn a kernel function in the form of a deep neural network, and then evaluate the MMD distance on a held-out test set (Liu et al., 2020). The test statistic can be chosen based on finite sample bounds or based on its asymptotic distribution (Gretton et al., 2012a) or nonparametric permutation tests (Liu et al., 2020). Lastly, the previous classifier two-sample tests can be represented as a special case of MMD (Liu et al., 2020).

Other shifts. In the context of *concept drift* (Gama et al., 2014), there has been work detecting shifts in $p(x, y)$ (Gonçalves Jr et al., 2014; Vovk, 2020). Harmful shifts can be detected as well (Podkopaev & Ramdas, 2021). However, these works assume that ground truth labels are provided for test examples, whereas our approach only requires unlabeled test examples. The former is substantially easier, since it suffices to check for drift in the distribution of prediction errors, which is usually very simple (e.g., a Bernoulli distri-

bution for the 0-1 loss), making it easy to test for drift. In contrast, our approach checks for drift in high-dimensional covariates distribution.

Sequential hypothesis testing. A closely related problem is sequential hypothesis testing, which adaptively decides whether to reject the null hypothesis as samples become available (Wald, 1945). These approaches can also be applied to two-sample testing (Balsubramani & Ramdas, 2015; Lhéritier & Cazals, 2018; 2019; Manole & Ramdas, 2021). However, as discussed above, they assume that each distribution of the two samples does not change over time. In contrast, we are interested in the setting where the test examples might initially be from the same distribution as the training examples, but then shift at a later point in time. Sequential tests are not applicable to this setting.

Change point detection. A related problem is change point detection (Page, 1954; Adams & MacKay, 2007; Boracchi et al., 2018; Volkhonskiy et al., 2017; Vovk et al., 2021), which detects the point at which a distribution changes. However, change point detection focuses on detecting a single shift, whereas our approach can detect gradual shifts.

3. Sequential Covariate Shift Detection

3.1. Problem Formulation

Let \mathcal{X} be the covariate space, \mathcal{S} be the source distribution over \mathcal{X} , and $\mathcal{T}_{t_s:t_e} = (\mathcal{T}_{t_s}, \mathcal{T}_{t_s+1}, \dots, \mathcal{T}_{t_e})$ be a sequence of target distributions over \mathcal{X} from time steps t_s to t_e . On time step t , we consider samples $x_t \sim \mathcal{S}$ and $x'_t \sim \mathcal{T}_t$; in practice, \mathcal{S} can be taken to be the uniform distribution over the training set. We let $S_{w,t} = (x_{t-w+1}, x_{t-w+2}, \dots, x_t)$ and $T_{w,t} = (x'_{t-w+1}, x'_{t-w+2}, \dots, x'_t)$ denote the recent examples in a time window of a given size $w \in \mathbb{N}$. Note that w can be different in source and target, but we use the same w for simplicity.

Our goal is to detect covariate shift at any step t . More precisely, we want to determine whether $\mathcal{S} \neq \bar{\mathcal{T}}_{w,t}$, where

$$\bar{\mathcal{T}}_{w,t} = \sum_{k=t-w+1}^t \frac{\mathcal{T}_k}{w}, \quad (1)$$

i.e., whether the average target distributions over the previous w steps is shifted compared to \mathcal{S} . For a fixed step t , this problem is a two-sample test (Lehmann & Romano, 2006), where the null hypothesis is $H_0 : \mathcal{S} = \bar{\mathcal{T}}_{w,t}$, and the alternative is $H_1 : \mathcal{S} \neq \bar{\mathcal{T}}_{w,t}$. That is, a two-sample test \hat{f} is designed to compute

$$\hat{f}(S_{w,t}, T_{w,t}) \approx \begin{cases} 1 & \text{if } \mathcal{S} \neq \bar{\mathcal{T}}_{w,t} \\ 0 & \text{otherwise.} \end{cases}$$

Our goal is to design a two-sample test \hat{f} for detecting covariate shift with this data stream. While we can in principle

use any two-sample test, our goal is to design one that is both sample and computationally efficient while achieving high accuracy for high-dimensional data such as images. In addition, we want the test \hat{f} to come with finite sample guarantees on the false positive rate. In particular, given $\alpha \in \mathbb{R}_{>0}$, if $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$, we want to ensure

$$\mathbb{P}_{S_{w,t} \sim \mathcal{S}^w, T_{w,t} \sim \mathcal{T}_{t-w+1:t}} \left[\hat{f}(S_{w,t}, T_{w,t}; \alpha) = 0 \right] \geq 1 - \alpha.$$

Ideally, we also want to provide finite sample bounds on the false negative rate; however, for classifier tests, we can only do so under additional assumptions about the model family used to try and distinguish \mathcal{S} and $\bar{\mathcal{T}}_{w,t}$. Intuitively, we assume that (i) the model family has bounded complexity (e.g., Rademacher complexity), and (ii) some model exists in the family that achieves nontrivial accuracy at distinguishing \mathcal{S} and $\bar{\mathcal{T}}_{w,t}$. Our goal is to ensure that if $\mathcal{S} \neq \bar{\mathcal{T}}_{w,t}$, then

$$\mathbb{P}_{\substack{S_{w,t} \sim \mathcal{S}^w, \\ T_{w,t} \sim \mathcal{T}_{t-w+1:t}}} \left[\hat{f}(S_{w,t}, T_{w,t}; \alpha) = 1 \right] \geq 1 - M(\alpha, w)$$

for $S^w = \mathcal{S} \times \dots \times \mathcal{S}$ consists of w copies of \mathcal{S} , and a function $M(\alpha, w)$ that depends on the model family.

3.2. Algorithm Overview

Next, we describe our two-sample test. We build on classifier two-sample test (C2ST) (Lopez-Paz & Oquab, 2017; Kim et al., 2021). The idea is to train a classifier \hat{g}_t to try and distinguish $S_{w,t}$ from $T_{w,t}$. Intuitively, if \mathcal{S} and $\bar{\mathcal{T}}_{w,t}$ are different distributions, then \hat{g}_t should achieve nontrivial accuracy at distinguishing $S_{w,t}$ from $T_{w,t}$ (assuming the model family is sufficiently expressive). Alternatively, if $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$, then \hat{g}_t necessarily achieves a trivial expected accuracy of 1/2.

In particular, the accuracy of \hat{g}_t can be used as a test statistic for the two-sample test. To choose the cutoff for rejecting the null hypothesis, we use the Clopper-Pearson (CP) interval (Clopper & Pearson, 1934) to construct an interval that contains the true accuracy \hat{g}_t with high probability based on the accuracy of \hat{g}_t on a test set. More precisely, the CP interval is an exact confidence interval around the empirical estimate of the mean of a Bernoulli random variable. Letting $z_1, \dots, z_n \sim \text{Bernoulli}(\mu^*)$ be i.i.d. samples from a Bernoulli distribution with true mean μ^* , the (unnormalized) estimate of its mean $n \cdot \hat{\mu}(z_{1:n}) = \sum_{i=1}^n z_i$ has distribution $\text{Binomial}(n, \mu^*)$. Then, the CP interval $\Theta_{\text{CP}}(\hat{s}, n; \alpha) \subseteq [0, 1]$ is an interval around $\hat{\mu}$ containing μ^* with probability at least $1 - \alpha$, *i.e.*,

$$\mathbb{P}_{\hat{s} \sim \text{Binomial}(n, \mu^*)} [\mu^* \in \Theta_{\text{CP}}(\hat{s}, n; \alpha)] \geq 1 - \alpha, \quad (2)$$

where the probability is taken over \hat{s} , α is a given confidence level, and Θ_{CP} is a function of the Binomial random variable

$\hat{s} = n \cdot \hat{\mu}(z_{1:n})$. The CP interval is concretely defined by

$$\Theta_{\text{CP}}(\hat{s}, n; \alpha) := \left[\inf \left\{ \theta \mid F(n - \hat{s}; n, 1 - \theta) \geq \frac{\alpha}{2} \right\}, \sup \left\{ \theta \mid F(\hat{s}; n, \theta) \geq \frac{\alpha}{2} \right\} \right],$$

where $F(s; n, \theta)$ is the cumulative distribution function (CDF) of Binomial(n, θ). To compute the CP interval, we can use the following equivalent formula:

$$\Theta_{\text{CP}}(\hat{s}, n; \alpha) = \left[Q \left(\frac{\alpha}{2}; \hat{s}, n - \hat{s} + 1 \right), Q \left(1 - \frac{\alpha}{2}; \hat{s} + 1, n - \hat{s} \right) \right],$$

where $Q(p, a, b)$ is the p th quantile of a Beta distribution with parameters a, b (Hartley & Fitch, 1951; Brown et al., 2001). Our algorithm uses the CP interval to determine whether the accuracy of \hat{g}_t is nontrivial, *i.e.*, $> 1/2$. In particular, the accuracy of \hat{g}_t is the mean of the Bernoulli random variable $\mathbb{1}(\hat{g}_t(x) = y)$, where y is the ground truth indicating whether x is from \mathcal{S} or $\bar{\mathcal{T}}_{w,t}$. Then, our algorithm rejects if the CP interval does not contain $1/2$, since this condition implies that the accuracy of \hat{g}_t does not equal $1/2$ with high probability. We describe this step in detail below.

The key challenge is what data to use as the test dataset to estimate the accuracy of \hat{g}_t . The traditional strategy is to split the available data into two parts: one to train \hat{g}_t and a second held-out test set to estimate its accuracy (Lopez-Paz & Oquab, 2017; Kim et al., 2021). However, this approach reduces sample efficiency, which is problematic in our setting since we often want w to be small.

To address this challenge, our algorithm exploits the conditional independence structure of classifier predictions. In particular, as described below, our algorithm uses each example x_t to evaluate the accuracy of \hat{g}_t *before* using it to train \hat{g}_t . In the next section, we prove that this strategy maintains the independence of our estimate of the accuracy of \hat{g}_t (Lemma 4.1), and that as a consequence, our algorithm satisfies the desired false positive rate (for a single step t).

3.3. Algorithm Details

Sequential detection algorithm. At each time step t , we observe a source sample $x_t \sim \mathcal{S}$ and a target sample $x'_t \sim \mathcal{T}_t$. In practice, we observe only new target samples, so we randomly draw source samples from the fixed set of source samples at each time step. By using these current samples and previous samples, we detect covariate shifts by updating the source-target classifier in online learning. In particular, our algorithm consists of three steps: (1) source-target prediction, (2) covariate shift detection, and (3) online source-

Algorithm 1 Sequential Calibrated Classifier Two-Sample Test

- 1: **Input:** significance level α , window size w
 - 2: **for** each time step t **do**
 - 3: Draw examples $x_t \sim \mathcal{S}, x'_t \sim \mathcal{T}_t$
 - 4: Predict $\hat{y}_t = \hat{g}_t(x_t)$ and $\hat{y}'_t = \hat{g}_t(x'_t)$
{▷ Source-target prediction}
 - 5: Detect covariate shift if $0.5 \notin \Theta_{\text{CP}}(2w\hat{\mu}_{w,t}, 2w; \alpha)$
{▷ Calibrated covariate shift detection}
 - 6: Update \hat{g}_t using $(x_t, 0)$ and $(x'_t, 1)$
{▷ Online source-target classifier update}
 - 7: **end for**
-

target classifier update. The following and Algorithm 1 include details.

Step 1. Source-target prediction. We predict source-target labels on the current samples x_t and x'_t using the current source-target classifier \hat{g}_t . In particular, we denote prediction on the source sample x_t by \hat{y}_t , *i.e.*, $\hat{y}_t = \hat{g}_t(x_t)$, and denote prediction on the target sample x'_t by \hat{y}'_t , *i.e.*, $\hat{y}'_t = \hat{g}_t(x'_t)$. These predictions and previous predictions are used in covariate shift detection in the following step.

Step 2. Calibrated covariate shift detection. Let $\mathcal{Q}_{w,t}$ be a distribution over $\mathcal{X} \times \{0, 1\}$, where

$$\mathcal{Q}_{w,t}(x, y) := \frac{1}{2} \cdot \mathcal{S}(x) \cdot \mathbb{1}(y = 0) + \frac{1}{2} \cdot \bar{\mathcal{T}}_{w,t}(x) \cdot \mathbb{1}(y = 1).$$

Then, $z = \mathbb{1}(\hat{g}_t(x) = y)$ is a Bernoulli random variable with distribution Bernoulli($\mu_{w,t}^*$), where

$$\mu_{w,t}^* = \mathbb{P}_{(x,y) \sim \mathcal{Q}_{w,t}}[\hat{g}_t(x) = y] \quad (3)$$

is the accuracy of \hat{g}_t at distinguishing whether an example x is from distribution \mathcal{S} or $\bar{\mathcal{T}}_{w,t}$. The unbiased empirical estimate of this accuracy is denoted by

$$\hat{\mu}_{w,t} = \frac{1}{2w} \sum_{i=t-w+1}^t (\mathbb{1}(\hat{y}_i = y_i) + \mathbb{1}(\hat{y}'_i = y'_i)).$$

In fact, $2w\hat{\mu}_{w,t}$ is a Binomial random variable with Binomial($2w, \mu_{w,t}^*$); thus, the accuracy $\mu_{w,t}^*$ can be estimated by the Clopper-Pearson (CP) interval $\Theta_{\text{CP}}(2w\hat{\mu}_{w,t}, 2w; \alpha)$ that includes the unknown parameter $\mu_{w,t}^*$ with high probability, *i.e.*,

$$\mathbb{P}[\mu^* \in \Theta_{\text{CP}}(2w\hat{\mu}_{w,t}, 2w; \alpha)] \geq 1 - \alpha.$$

This property can be used for checking the accuracy of \hat{g}_t might be $1/2$. In particular, our algorithm returns “covariate shift” if $1/2 \notin \Theta_{\text{CP}}(2w\hat{\mu}_{w,t}, 2w; \alpha)$, and “no covariate shift” otherwise, *i.e.*

$$\hat{f}(S_{w,t}, T_{w,t}; \alpha) = \mathbb{1} \left(\frac{1}{2} \notin \Theta_{\text{CP}}(2w \cdot \hat{\mu}_{w,t}, 2w; \alpha) \right).$$

Here, the Clopper-Pearson interval calibrates the empirical accuracy $\hat{\mu}_{w,t}$ using the property of the Binomial distribution.

Step 3. Online source-target classifier update. Finally, we update a binary classifier \hat{g}_t using new training examples based on the source and target samples, *i.e.*, $(x_t, 0)$ and $(x'_t, 1)$. In general, \hat{g}_t can be any model; we consider it to be a neural network, in which case we can update its parameters using stochastic gradient descent with respect to the cross entropy loss.

4. Theoretical Guarantees

In this section, we describe our finite sample bounds on the false positive and false negative rates of our covariate shift detector \hat{f} ; the key to have valid bounds is proving the independence on predictions $\hat{y}_1, \dots, \hat{y}_t$ (and $\hat{y}'_1, \dots, \hat{y}'_t$) to have a valid Clopper-Pearson interval, since they are seemingly dependent through the online learned classifier \hat{g}_t . First, our key result shows that our estimate of the accuracy of \hat{g}_t is valid—*i.e.*, the predictions $\hat{y}_i, \dots, \hat{y}_j$ are conditionally independent (see Appendix A.1 for a proof), thus the accuracy is the parameter of the Binomial distribution:

Lemma 4.1. *If x_i, \dots, x_j are independent for any $i, j \in \mathbb{N}$ where $i < j$, $\hat{y}_i, \dots, \hat{y}_j$ are conditionally independent given $\hat{g}_i, \dots, \hat{g}_{j-1}$.*

Our next result says that our algorithm ensures the desired bound α on the false positive rate (*i.e.*, \hat{f} says “covariate shift” when there is no covariate shift). To this end, we exploit the following observation that *any* source-target classifier makes the expected accuracy of $1/2$ if there is no covariate shift. Intuitively, if $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$, source-target classification is impossible (Lopez-Paz & Oquab, 2017; Liu et al., 2020); we include this lemma for completeness (see Appendix A.2 for a proof):

Lemma 4.2. *Define $\bar{\mathcal{T}}_{w,t}$ as in Eq. (1) and $\mu_{w,t}^*$ as in Eq. (3). If $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$, we have $\mu_{w,t}^* = 1/2$ for any source-target classifier \hat{g}_t .*

Since the expected accuracy of \hat{g}_t is $1/2$ regardless of how we design and learn \hat{g}_t , and how many samples are used to learn \hat{g}_t , the Clopper-Pearson interval includes the true accuracy with high probability; thus the false positive rate of the proposed covariate shift detector \hat{f} is effectively controlled by the confidence level of the Clopper-Pearson interval, as follows (see Appendix A.3 for a proof):

Theorem 4.3 (Bound on false positive rate). *Define $\bar{\mathcal{T}}_{w,t}$ as in Eq. (1). If $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$, for any source-target classifier \hat{g}_t , we have*

$$\mathbb{P}_{(S_{w,t}, T_{w,t}) \sim \mathcal{S}^w \times \mathcal{T}_{t-w+1:t}} \left[\hat{f}(S_{w,t}, T_{w,t}; \alpha) = 0 \right] \geq 1 - \alpha. \quad (4)$$

Note that our FPR bound is not time-uniform; we can obtain time-uniform bounds by taking α to zero sufficiently quickly; please refer to discussion in Appendix B.2.

Our next result provides a bound on the false negative rate; we first observe that the Clopper-Pearson interval is included in the interval by the Hoeffding’s bound. Intuitively, the Clopper-Pearson interval represents a lower and upper bound of the expected accuracy given an empirical accuracy tailored to a Bernoulli random variable; the Hoeffding’s bound can similarly bound the mean but in a more general setup. Thus, the Clopper-Pearson interval can be smaller (see Appendix A.4 for a proof).

Lemma 4.4. *Let $s \sim \text{Binomial}(n, p)$ and $F(s; n, p)$ is the CDF of Binomial(n, p); we have*

$$\frac{s}{n} - \sqrt{\frac{\ln \frac{2}{2n}}{2n}} \leq \inf \left\{ \theta \mid F(n - s; n, 1 - \theta) \geq \frac{\alpha}{2} \right\} \text{ and}$$

$$\sup \left\{ \theta \mid F(s; n, \theta) \geq \frac{\alpha}{2} \right\} \leq \frac{s}{n} + \sqrt{\frac{\ln \frac{2}{2n}}{2n}}.$$

Leveraging this, we have the following bound on false negative rate (see Appendix A.5 for a proof).

Theorem 4.5 (Bound on false negative rate). *Define $\bar{\mathcal{T}}_{w,t}$ as in Eq. (1) and $\mu_{w,t}^*$ as in Eq. (3). Assume a source-target classifier \hat{g}_t achieves nontrivial accuracy, *i.e.*, $\mu_{w,t}^* \geq 1/2 + \epsilon$, where $\epsilon \in (0, 1/2]$, is the accuracy at distinguishing \mathcal{S} and $\bar{\mathcal{T}}_{w,t}$. Let $a(w, \alpha) := 2w(1/2 + \sqrt{\log(2/\alpha)/4w})$ and $b(w, \alpha) := 2w(1/2 - \sqrt{\log(2/\alpha)/4w})$. If $\mathcal{S} \neq \bar{\mathcal{T}}_{w,t}$ and $w - 1 - \lfloor \sqrt{w \log(2/\alpha)} \rfloor \geq 0$, then we have*

$$\mathbb{P} \left[\hat{f}(S_{w,t}, T_{w,t}; \alpha) = 1 \right]$$

$$\geq F \left(2w - \lfloor a(w, \alpha) + 1 \rfloor; 2w, \frac{1}{2} - \epsilon \right)$$

$$+ F \left(\lceil b(w, \alpha) - 1 \rceil; 2w, 1 \right).$$

In the false negative bound, the first term is dominant and increases as w increases, which implies the sample size needs to be increased to have a powerful shift detector; the condition on w suggests that the bound is valid when $w \geq 201$ given $\alpha = 0.01$. This theorem provides a partial answer to the cold start performance which any test can suffer from. To practically use our algorithm, we need to know the amount of samples for a reliable detection. This FNR bound offers a guideline for the required number of samples for the given magnitude under certain assumptions. We note that the assumption $L(\hat{g}_t) := 1 - \mu^* \leq 1/2 - \epsilon$ can be achieved under standard conditions. For instance, assume that the model family \mathcal{G} of source-target classifiers has finite VC dimension (*i.e.*, $\text{VC}(\mathcal{G}) < \infty$), and that the optimal model $g^* \in \mathcal{G}$ has nontrivial inaccuracy $L(g^*) = 1/2 - \xi$

for some $\xi \in \mathbb{R}_{>0}$; then, with probability at least $1 - \delta$ with respect to $S_{w,t}$ and $T_{w,t}$ and letting $m = 2w$, we have

$$\begin{aligned} L(\hat{g}_t) &\leq L(g^*) + 4\sqrt{\frac{\text{VC}(\mathcal{G})(\log(2m) + 1)}{m}} + \sqrt{\frac{\log(2/\delta)}{m}} \\ &\leq \frac{1}{2} - \underbrace{\left(\xi - 4\sqrt{\frac{\text{VC}(\mathcal{G})(\log(2m) + 1)}{m}} - \sqrt{\frac{\log(2/\delta)}{m}} \right)}_{=:\epsilon}, \end{aligned}$$

where the second term (which we have taken to be ϵ) satisfies $\epsilon > 0$ for sufficiently large m (Vapnik, 1998).

5. Experiments

We evaluate the effectiveness of our algorithm at detecting both natural and synthetic covariate shifts of varying forms (e.g., gradual shifts and multiple shifts back and forth), showing that it significantly outperforms natural baselines. In this section, we show the experimental results on ImageNet; see Appendix C for the results on IWildCam and Py150. We have released our code for these experiments.¹

5.1. Experiment Setup

Baselines. We compare our algorithm to six baselines; two of them differ in the way they use the samples at each time step, the third uses Wald’s sequential likelihood test (Wald, 1945), the fourth one is based on DeepKernel (Liu et al., 2020), the fifth one is based on KD-Switch (Lh eritier & Cazals, 2019), and the last one is based on inductive conformal martingales (Volkhonskiy et al., 2017; Eliades & Papadopoulos, 2021). For the first two baselines, while our approach uses all samples to construct the CP interval around the accuracy of the source-target classifier \hat{g}_t as well as to train \hat{g}_t , the baseline instead constructs a held-out test set using every H^{th} sample. Then, only this held-out test set is used to compute the CP interval, and only the remaining samples are used to train \hat{g}_t . In our experiments, we used values of $H \in \{2, 5\}$, denoted H2, H5, respectively. For Wald’s test, we consider the Bernoulli random variable with a probability p indicating whether the prediction of the source-target classifier is correct for the given sample. The hypothesis test is $H_0 : p = 0.5$ vs. $H_1 : p = 0.5 + \epsilon$, where $\epsilon = 0.2$ in our experiments; we restart the test each time it makes a decision. For Deep Kernel (DK), since it requires training of the kernel parameters and the network for extracting features, we use half of the samples for this training process and conduct the test using the remaining ones. For KD-Switch (KDS), we also restart the test when it makes a decision as we do for Wald’s test. The last baseline,

inductive conformal martingale (ICM), uses source-target classifier’s output as non-conformity score and a constant betting function.

H2 and H5 are the online version of an existing classifier two-sample test (C2ST) (Kim et al., 2021; Lopez-Paz & Oquab, 2017), which splits the (fixed) training dataset into a training set to train \hat{g}_t and a held-out test set to estimate the accuracy of \hat{g}_t ; thus, H controls the tradeoff between the number of examples in the training set and held-out test set.

Source-target classifier. We use a fully-connected neural network with a single hidden layer (with 128 hidden units) and with the ReLU activation functions as the source-target classifier \hat{g}_t . We use a binary cross-entropy loss for training in conjunction with an SGD optimizer with a learning rate of 0.01 (for natural shift experiments) and 0.001 (for synthetic shift experiments). Finally, since the inputs are ImageNet images (Russakovsky et al., 2015), we use a 2048-dimensional feature vector generated by first running a pretrained ResNet152 model (He et al., 2016) on the images, and then using these features vectors for the covariates of $S_{w,t}$ and $T_{w,t}$.

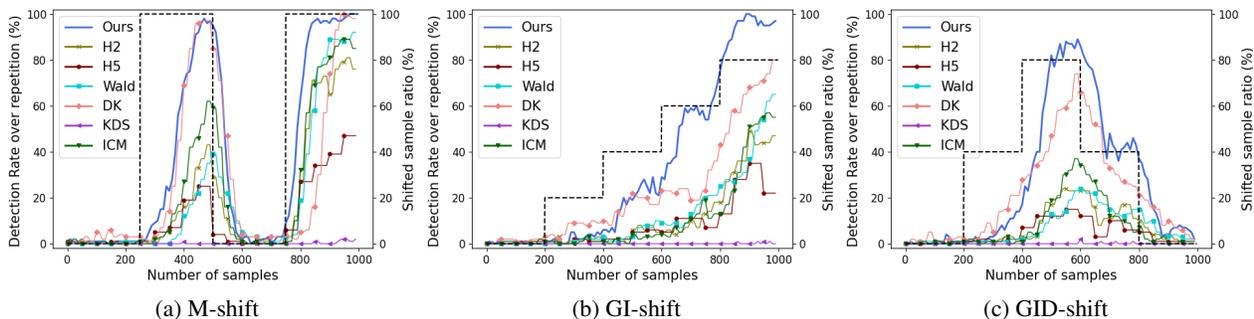
Scenarios. We run each algorithm to test whether the target distribution in the given window is shifted with three different scenarios: multiple shift (“M-shift”), gradually increasing shift (“GI-shift”), and gradually increasing-then-decreasing shift (“GID-shift”). Table 1 describes each scenario. For example, the multiple shift scenario proceeds as follows: (i) it starts with no covariate shift at the beginning; (ii) after observing 25% target samples (i.e., 250th samples for natural shift experiments and 2500th samples for synthetic shift experiments), covariate shift is applied to all target samples (with probability 1) by adding random perturbations for synthetic shift and by drawing samples from a target distribution for natural shift; (iii) after 50% of target samples, it reverts to no covariate shift; and (iv) finally after observing 75% target samples, the covariate shift is applied to the all target samples. Gradually increasing shift and gradually increasing-then-decreasing shift scenarios start with no covariate shift for the first 20% of target samples; then, covariate shift is applied with some probability $0 < p < 1$ by gradually changing p over time.

Stream data generation. For each shift (i.e., natural shift and synthetic shift), we have a source dataset \mathcal{S} and target datasets \mathcal{T}_t , from which we randomly draw source and target samples for each time step t . In particular, we consider a batch of samples for computational efficiency, where we denote the batch size by B ; we use $B = 10$ for our experiments. That is, we wait for B samples to be collected from the target distribution before checking for covariate shift and the updating the source-target classifier; then, we begin collecting the next batch. Finally, we evaluate each approach using multiple random repetitions, which we denote by R

¹https://github.com/sooyongj/sequential_covariate_shift_detection

Table 1: Scenario description for experiments. (a) ‘‘M-shift’’ is Multiple shift, (b) ‘‘GI-shift’’ is gradually increasing shift, and (c) ‘‘GID-shift’’ is gradually increasing-then-decreasing shift.

(a) M-shift			(b) GI-shift			(c) GID-shift		
Start position	Description	Prob.	Start position	Description	Prob.	Start position	Description	Prob.
0%	No shift	0.0	0%	No shift	0.0	0	No shift	0.0
25%	Shift	1.0	20%	Shift	0.2	20%	Shift	0.4
50%	No shift	0.0	40%	Shift	0.4	40%	Shift	0.8
75%	Shift	1.0	60%	Shift	0.6	60%	Shift	0.4
			80%	Shift	0.8	80%	No shift	0.0


 Figure 1: Detection rate for natural shift with $R = 100$, $w = 10$, $\alpha = 1\%$. The black dashed line indicates shifted sample ratio, *i.e.*, the degree (or probability) of covariate shift.

(the value of R depends on each experiment).

5.2. Natural shift

Dataset. First, we consider a natural shift on ImageNet. To construct such a shift, we consider the subset of dog classes; in particular, 120 of the 1000 of the ImageNet classes are of dogs (Khosla et al., 2011). Then, we randomly select half (*i.e.*, 60) of these classes to be the source dataset, and the other half to be the target dataset; thus, the number of source and target images is 2997 each (after removing duplicated images). As a consequence, the source and target datasets correspond to different dog breeds, which is a kind of natural distribution shift.

Results. Figure 1 and Table 2 show results for the natural shift experiment with $w = 10$ and $\alpha = 1\%$. Figure 1 illustrates detection rates of the seven algorithms with $R = 100$ repetitions (*i.e.*, the fraction of repetitions that reported ‘‘covariate shift’’ at each step). Table 2a shows the number of shifted samples required to reach at least 80% of covariate shift detection rate under the shift. Table 2b shows false positive rate (FPR) after 50, 100, 150, and 200 samples with $R = 20000$ repetitions.

Discussion. Figure 1 shows the detection rate of each algorithm as each scenario progresses. In multiple shift (Figure 1a) and gradually increasing-then-decreasing shift (Figure

 Table 2: Natural shift results with (a) $w = 10$, $\alpha = 1\%$, and $R = 100$, and (b) $R = 20000$ ². In (a), we bold the best algorithm and underline the second-best algorithm. In (b), we bold values that violate the desired $\alpha = 1\%$.

(a) Number of samples for detection ($\geq 80\%$)			(b) FPR (%) at selected time					
Scn.	Alg.	Natural shift	Scn.	Alg.	50	100	150	200
M-shift	Ours	<u>190</u>	M-shift	Ours	0.27	0.53	0.73	0.77
	H2	720		H2	0.29	0.28	0.26	0.33
	H5	-		H5	0.34	0.52	0.51	0.56
	Wald	640		Wald	0.60	0.47	0.27	0.27
	DK	180		DK	1.69	2.31	2.16	2.54
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	660		ICM	0.21	0.18	0.27	0.19
GI-shift	Ours	620	GI-shift	Ours	0.21	0.60	0.76	0.83
	H2	-		H2	0.21	0.25	0.29	0.36
	H5	-		H5	0.32	0.43	0.50	0.85
	Wald	-		Wald	0.78	0.57	0.29	0.22
	DK	<u>790</u>		DK	2.11	2.67	2.22	3.29
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.22	0.22	0.18	0.19
GID-shift	Ours	310	GID-shift	Ours	0.30	0.53	0.70	0.95
	H2	-		H2	0.18	0.21	0.28	0.41
	H5	-		H5	0.36	0.56	0.53	0.81
	Wald	-		Wald	0.77	0.58	0.34	0.23
	DK	-		DK	1.91	2.67	2.37	3.42
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.29	0.23	0.20	0.20

²We use $R = 100$ for KDS as it is computationally expensive.

1c), covariate shift disappears after a certain point, all algorithms correctly detect this change. However, as shown

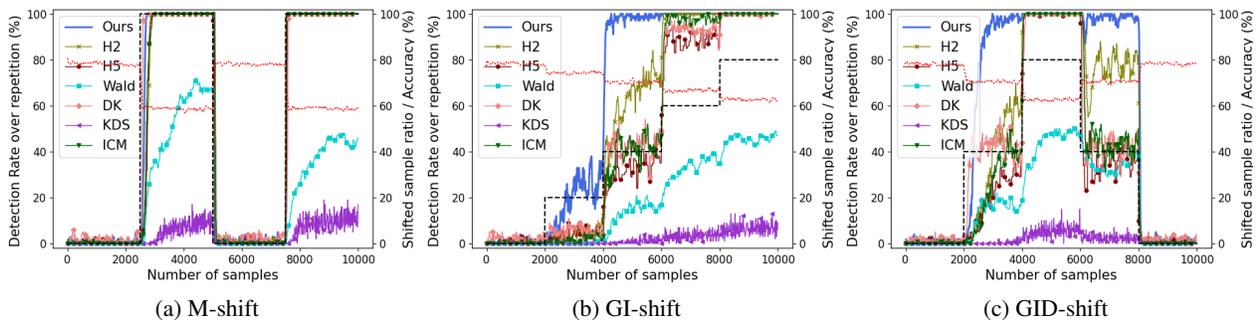


Figure 2: Detection rate for synthetic shifts with Gaussian noise perturbation, Severity = 2, $R = 100$, $w = 10$, $\alpha = 1\%$. The black dashed line indicates shifted sample ratio, *i.e.*, the degree (or probability) of covariate shift. The red dotted line shows the accuracy of ResNet152 on the source and target samples in the given window.

Table 3: Synthetic shift results with (a) Severity = 2, $w = 10$, $\alpha = 1\%$, and $R = 100$, and (b) $R = 20000^3$. In (a), we bold the best algorithm and underline the second-best algorithm. In (b), we bold values that exceed the desired $\alpha = 1\%$.

(a) Number of samples for detection							(b) FPR (%) at selected time					
Scenario	Alg.	Contrast	Defocus Blur	Elastic Transform	Gaussian Blur	Gaussian Noise	Scenario	Alg.	500	1000	1500	2000
M-shift	Ours	230	<u>200</u>	<u>220</u>	<u>210</u>	<u>180</u>	M-shift	Ours	0.75	0.99	0.95	0.97
	H2	470	450	450	490	350		H2	0.41	0.46	0.46	0.52
	H5	410	410	410	460	310		H5	0.78	0.73	0.85	0.67
	Wald	-	-	-	-	-		Wald	0.07	0.11	0.04	0.01
	DK	150	90	110	90	110		DK	2.08	2.07	1.94	2.17
	KDS	-	-	-	-	-		KDS	0.00	0.00	0.00	0.01
	ICM	410	290	370	330	310		ICM	0.24	0.22	0.24	0.19
GI-shift	Ours	2100	2060	2090	2070	2080	GI-shift	Ours	0.86	0.89	0.92	0.85
	H2	<u>4050</u>	3690	<u>4050</u>	<u>4010</u>	<u>3670</u>		H2	0.62	0.54	0.60	0.50
	H5	4360	4110	6010	4110	4110		H5	0.74	0.71	0.77	0.73
	Wald	-	-	-	-	-		Wald	0.10	0.13	0.07	0.03
	DK	6130	<u>2210</u>	4130	4090	4110		DK	2.04	2.08	1.93	2.14
	KDS	-	-	-	-	-		KDS	0.00	0.00	0.00	0.00
	ICM	4070	4070	4090	4070	4070		ICM	0.18	0.16	0.15	0.22
GID-shift	Ours	880	<u>560</u>	900	720	610	GID-shift	Ours	0.87	0.95	0.92	0.89
	H2	2030	2010	2050	2010	2010		H2	0.51	0.57	0.51	0.53
	H5	2060	2060	2060	2060	2060		H5	0.73	0.75	0.85	0.89
	Wald	-	-	-	-	-		Wald	0.09	0.08	0.04	0.02
	DK	2170	190	2070	2050	2070		DK	2.05	2.05	2.04	2.13
	KDS	-	-	-	-	-		KDS	0.01	0.00	0.00	0.00
	ICM	2050	2030	<u>2050</u>	2030	2030		ICM	0.17	0.23	0.15	0.22

in Table 2a, our approach always requires fewer samples to detect the shift, except for M-shift, where DK slightly outperforms it (at the cost of an excessive FPR, as discussed below). Whereas H5, KDS do not achieve 80% detection, H2, Wald, DK, and ICM reach 80% only for some scenarios, our approach always detects covariate shift at a rate higher than 80%. Furthermore, for multiple shift, our algorithm requires similar or fewer than half the number of samples compared to H2, Wald, DK, and ICM. In summary, our algorithm is significantly more sample efficient at detecting covariate shift compared to the baselines, most likely since it utilizes all samples for both training the source-target classifier and constructing the CP interval. For FPR, all algorithms except DK always satisfy the FPR bound (*i.e.*, $FPR \leq \alpha$).

5.3. Synthetic shift

Dataset. Next, we consider a synthetic shift on ImageNet. In particular, we split the original ImageNet validation set into equal sized source and target datasets. To construct the target dataset, we add synthetic perturbations on original images. We (separately) consider five perturbation types from Hendrycks & Dietterich (2019)—in particular, Contrast, Defocus Blur, Elastic Transform, Gaussian Blur, and Gaussian Noise, with five different severity levels.

Results. The experiment results are shown in Figure 2 and Table 3 for the experiments with the perturbation severity of 2, window size $w = 10$, and significance level $\alpha =$

³We use $R = 100$ for KDS as it is computationally expensive.

1%. Table 3a shows the number of target samples required by each algorithm to detect the first covariate shift in the detection rate of at least 80%. Table 3b shows the false positive rate (FPR) after 500, 1000, 1500 and 2000 samples for each of the three scenarios. Figure 2 shows the detection rates over multiple repetitions for each of the three scenarios using the Gaussian noise perturbation. Results for other perturbation types and severities are shown in Appendix C.

Discussion. As can be seen, our approach outperforms the baselines in terms of sample efficiency for the covariate shift detection as was the case of the natural shift. The only exceptions are M-shift and Defocus Blur in the GID-shift scenario, where the difference is not large compared to other algorithms. Our algorithm requires about half as many samples before detecting covariate shift compared to the baselines. In terms of FPR, our approach always satisfies the FPR bound. Finally, Figure 2 shows the accuracy drop with the shifted samples. In particular, the red dotted line shows the accuracy of ResNet152 on the examples in the source and target samples of the given window; as can be seen, the accuracy decreases as the degree of the shift increases. Covariate shift detection can be successfully used to notify a user that an accuracy drop may have occurred.

6. Conclusion

We have proposed a novel covariate shift detection algorithm, which uses a classifier two-sample test to check whether the current test examples differ in distribution compared to the training examples. Our approach ensures sample efficiency by avoiding the need to split the dataset into a training set and a held-out test set, and instead using all the data to both train the source-target discriminator and to evaluate its accuracy. We prove that even with this optimization, our approach provides finite sample guarantees on the false positive rate at a desired level; we also prove bounds on the false negative rate under a mild conditions on the trained classifier. Finally, we empirically demonstrate that our proposed algorithm is significantly more sample efficient compared to several baselines at detecting both natural and synthetic shifts on ImageNet.

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A. Proofs

A.1. Proof of Lemma 4.1

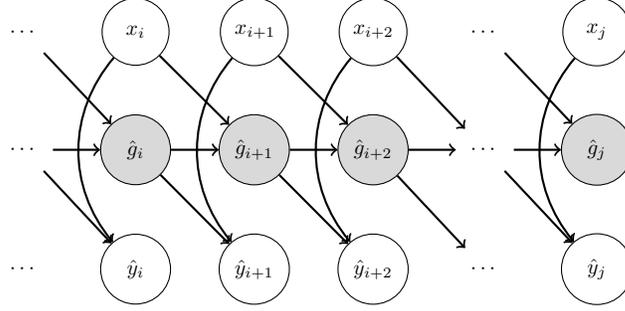


Figure 3: The dependency structure of random variables.

Figure 3 represents the graphical model over random variables, where observed random variables are colored in gray. We prove the conditional independence using the d-separation (also called the Bayes ball algorithm) (Bishop, 2006), which is a set of rules that can determine the conditional dependency between two random variables based on the graphical model and observed random variables. In particular, \hat{y}_{i+2} is conditionally independent to \hat{y}_k for all $k \leq i+1$ since the path to \hat{y}_k is blocked by \hat{g}_{i+1} (i.e., \hat{g}_{i+1} is observed). Similarly, \hat{y}_{i+2} is conditionally independent to \hat{y}_k for all $k \geq i+3$. This proves the claim. \square

A.2. Proof of Lemma 4.2

For any source-target classifier \hat{g}_t , if $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$, the following holds:

$$\begin{aligned}
 \mu_{w,t}^* &= \mathbb{P}_{(x,y) \sim \mathcal{Q}_{w,t}} [\hat{g}_t(x) = y] \\
 &= \int \sum_{y \in \{0,1\}} \mathbb{1}(\hat{g}_t(x) = y) \mathcal{Q}_{w,t}(x, y) dx \\
 &= \int \sum_{y \in \{0,1\}} \mathbb{1}(\hat{g}_t(x) = y) \left(\frac{1}{2} \cdot \mathcal{S}(x) \cdot \mathbb{1}(y=0) + \frac{1}{2} \cdot \bar{\mathcal{T}}_{w,t}(x) \cdot \mathbb{1}(y=1) \right) dx \\
 &= \frac{1}{2} \int \sum_{y \in \{0,1\}} \mathbb{1}(\hat{g}_t(x) = y) \mathcal{S}(x) \mathbb{1}(y=0) + \sum_{y \in \{0,1\}} \mathbb{1}(\hat{g}_t(x) = y) \bar{\mathcal{T}}_{w,t}(x) \mathbb{1}(y=1) dx \\
 &= \frac{1}{2} \int \mathbb{1}(\hat{g}_t(x) = 0) \mathcal{S}(x) + \mathbb{1}(\hat{g}_t(x) = 1) \bar{\mathcal{T}}_{w,t}(x) dx \\
 &= \frac{1}{2} \int \mathbb{1}(\hat{g}_t(x) = 0) \mathcal{S}(x) + \mathbb{1}(\hat{g}_t(x) = 1) \mathcal{S}(x) dx \\
 &= \frac{1}{2} \int (\mathbb{1}(\hat{g}_t(x) = 0) + \mathbb{1}(\hat{g}_t(x) = 1)) \mathcal{S}(x) dx \\
 &= \frac{1}{2} \int \mathcal{S}(x) dx \\
 &= \frac{1}{2},
 \end{aligned}$$

where the sixth equality holds since $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$; the claim follows. \square

A.3. Proof of Theorem 4.3

Denote the event that $\mathbb{P}_{(x,y) \sim \mathcal{Q}_{w,t}} [\hat{g}_t(x) = y] = 1/2$ by E , and let $\hat{s}_{w,t} = 2w\hat{\mu}_{w,t}$. Then, we have

$$\begin{aligned}
 & \mathbb{P}_{S_{w,t}, T_{w,t}} [\hat{f}(S_{w,t}, T_{w,t}; \alpha) = 0] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\left(\frac{1}{2} \in \Theta_{\text{CP}}(\hat{s}_{w,t}, 2w; \alpha) \right) \wedge \left(\mathbb{P}_{x,y} [\hat{g}_t(x) = y] = \frac{1}{2} \right) \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} [E] \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\frac{1}{2} \in \Theta_{\text{CP}}(\hat{s}_{w,t}, 2w; \alpha) \mid E \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\frac{1}{2} \in \Theta_{\text{CP}}(\hat{s}_{w,t}, 2w; \alpha) \mid E \right] \\
 &\geq 1 - \alpha,
 \end{aligned}$$

where the first equality holds since $\mathcal{S} = \bar{\mathcal{T}}_{w,t}$ and by Lemma 4.2, the third equality holds by Lemma 4.2, and the last inequality holds by the property of the Clopper-Pearson interval and Lemma 4.1. \square

A.4. Proof of Lemma 4.4

We use the tail bound of the binomial distribution using the Hoeffding's inequality—*i.e.*

$$F(s; n, p) \leq \exp \left\{ -2n \left(p - \frac{s}{n} \right)^2 \right\}.$$

For the upper bound of the upper Clopper-Pearson interval, we have

$$\begin{aligned}
 \sup \left\{ \theta \mid F(s; n, \theta) \geq \frac{\alpha}{2} \right\} &\leq \sup \left\{ \theta \mid \exp \left\{ -2n \left(\theta - \frac{s}{n} \right)^2 \right\} \geq \frac{\alpha}{2} \right\} \\
 &= \sup \left\{ \theta \mid \frac{s}{n} - \sqrt{\frac{\ln \frac{2}{\alpha}}{2n}} \leq \theta \leq \frac{s}{n} + \sqrt{\frac{\ln \frac{2}{\alpha}}{2n}} \right\} \\
 &= \frac{s}{n} + \sqrt{\frac{\ln \frac{2}{\alpha}}{2n}}.
 \end{aligned} \tag{5}$$

For the lower bound of the lower Clopper-Pearson interval, we have

$$\begin{aligned}
 \inf \left\{ \theta \mid F(n-s; n, 1-\theta) \geq \frac{\alpha}{2} \right\} &\geq \inf \left\{ \theta \mid \exp \left\{ -2n \left(\theta - \frac{s}{n} \right)^2 \right\} \geq \frac{\alpha}{2} \right\} \\
 &= \inf \left\{ \theta \mid \frac{s}{n} - \sqrt{\frac{\ln \frac{2}{\alpha}}{2n}} \leq \theta \leq \frac{s}{n} + \sqrt{\frac{\ln \frac{2}{\alpha}}{2n}} \right\} \\
 &= \frac{s}{n} - \sqrt{\frac{\ln \frac{2}{\alpha}}{2n}}.
 \end{aligned} \tag{6}$$

Finally, (5) and (6) imply the claim. \square

A.5. Proof of Theorem 4.5

Let the lower and upper bound of the Clopper-Pearson interval Θ_{CP} be $\underline{\Theta}_{\text{CP}}$ and $\overline{\Theta}_{\text{CP}}$, respectively. Recall that we denote the CDF of a binomial distribution $\text{Binomial}(n, p)$ by $F(s; n, p)$. Then, we have

$$\begin{aligned}
 & \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\hat{f}(S_{w,t}, T_{w,t}; \alpha) = 1 \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\frac{1}{2} \notin \Theta_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\left(\mu_{w,t}^* < \frac{1}{2} + \epsilon \vee \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right) \wedge \left(\frac{1}{2} \notin \Theta_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) \right) \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\left(\mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right) \wedge \left(\frac{1}{2} \notin \Theta_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) \right) \right] \tag{7}
 \end{aligned}$$

$$\begin{aligned}
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\frac{1}{2} \notin \Theta_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\frac{1}{2} \notin \Theta_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \tag{8} \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\underline{\Theta}_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) > \frac{1}{2} \vee \overline{\Theta}_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) < \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 &= \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\underline{\Theta}_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) > \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 &\quad + \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\overline{\Theta}_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) < \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right],
 \end{aligned}$$

where (7) and (8) hold due to $\mathbb{P}_{S_{w,t}, T_{w,t}}[\mu_{w,t}^* < 1/2 + \epsilon] = 0$ and $\mathbb{P}_{S_{w,t}, T_{w,t}}[\mu_{w,t}^* \geq 1/2 + \epsilon] = 1$ from the assumption on \hat{g}_t and $S \neq \bar{T}_{w,t}$, respectively.

By Lemma 4.4, the first term is lower bounded as follows:

$$\begin{aligned}
 & \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\underline{\Theta}_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) > \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & \geq \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\hat{\mu}_{w,t} - \sqrt{\frac{\ln \frac{2}{\alpha}}{4w}} > \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & = \mathbb{P}_{S_{w,t}, T_{w,t}} \left[2w\hat{\mu}_{w,t} > a(w, \alpha) \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & = \mathbb{P}_{S_{w,t}, T_{w,t}} \left[2w\hat{\mu}_{w,t} \geq \lfloor a(w, \alpha) + 1 \rfloor \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & \geq F \left(2w - \lfloor a(w, \alpha) + 1 \rfloor; 2w, \frac{1}{2} - \epsilon \right), \tag{9}
 \end{aligned}$$

where the last inequality holds since the binomial parameter $\frac{1}{2} - \epsilon$ makes the CDF F smallest.

Similarly, the second term is lower bounded as follows:

$$\begin{aligned}
 & \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\overline{\Theta}_{\text{CP}}(2w\mu_{w,t}^*, 2w; \alpha) < \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & \geq \mathbb{P}_{S_{w,t}, T_{w,t}} \left[\hat{\mu}_{w,t} + \sqrt{\frac{\ln \frac{2}{\alpha}}{4w}} < \frac{1}{2} \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & = \mathbb{P}_{S_{w,t}, T_{w,t}} \left[2w\hat{\mu}_{w,t} < b(w, \alpha) \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & = \mathbb{P}_{S_{w,t}, T_{w,t}} \left[2w\hat{\mu}_{w,t} \leq \lceil b(w, \alpha) - 1 \rceil \mid \mu_{w,t}^* \geq \frac{1}{2} + \epsilon \right] \\
 & \geq F(\lceil b(w, \alpha) - 1 \rceil; 2w, 1),
 \end{aligned} \tag{10}$$

where the last inequality holds since the binomial parameter $\mu_{w,t}^* = 1$ makes the CDF F smallest.

The claim follows by combining (9) and (10). \square

B. Additional Discussion

B.1. Multiple Epochs in Training

As shown in Algorithm 1, each example is used only once in updating the source-target classifier, baselines also follow this setting in all experiments. We consider this single epoch update anticipating that our algorithms being used in the online setting, where it is infeasible to take multiple passes over the training data. However, without consideration of the online setting, each example can be used multiple times during training with the restriction that the example can be used only once in the CP interval, which can improve the performance. As this strategy is orthogonal to our approach, it can be applied to both ours and other baselines expecting the performance improvement.

B.2. Time-uniform bound

Our notions of FPR and FNR (e.g., in Thm. 4.3) are for a single, fixed t . We make this choice since we expect covariate shift algorithms to run in production for extended periods of time, making it impractical to provide guarantees that hold uniformly across time. Then, our approach bounds the rate at which false positives occur. In principle, we can achieve a uniform bound by taking α to zero over time. For instance, to obtain a uniform bound of α , we can take $\alpha_t = (6/\pi^2) \cdot \alpha/t^2$ on step t (since $\sum_{t=1}^{\infty} 1/t^2 = \pi^2/6$).

C. Additional Experimental Results

C.1. Natural shift - IWILDcam

Dataset. In addition to ImageNet, we perform additional natural shift experiments on another image dataset, IWILDcam from WILDS dataset (Koh et al., 2021). WILDS dataset is a collection of datasets for distribution shift research and IWILDcam is one of such datasets which includes animal photos taken from different locations. This IWILDcam has two different test sets; denoted by Test (ID) and Test (OOD). Test (ID) is a collection of photos taken at the same locations as a training set while Test (OOD) is from the different locations. We consider the shift from Test (ID) to Test (OOD) as a natural covariate shift.

Source-target classifier. We use the same source-target classifier setting as we do for ImageNet natural shift experiments in terms of network architecture, loss, and learning rate. However, we use different model to extract features from IWILDcam images. We obtain the pretrained ResNet50 model, provided by the authors of the WILDS dataset paper (Koh et al., 2021), and run the model for the feature extraction.

Results. The results are shown in Figure 4 and Table 4. Figure 4 displays the detection rate and Table 4 shows the number of samples for detection ($\geq 80\%$) and FPR at selected time points.

Discussion. The results are similar to other two experiments in the main paper. As shown in Figure 4 and Table 4, most algorithms correctly react to the shifts, but our algorithm requires the smallest number of samples for detection. In addition, all algorithms except DK satisfy the FPR bound.

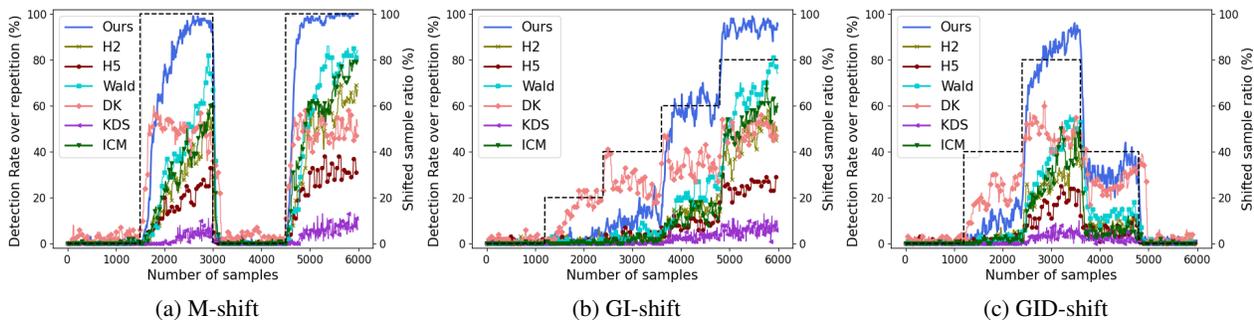


Figure 4: Detection rate for natural shift on IWildCam with $R = 100$, $w = 10$, $\alpha = 1\%$. The black dashed line indicates shifted sample ratio, *i.e.*, the degree (or probability) of covariate shift. Our approach achieves the high detection rate ($\geq 80\%$) with the smallest number of samples when covariate shift occurs. DK reaches the higher detection rate at the early stage of covariate shift, which may be caused by the higher FPR (Table 4b).

Table 4: Natural shift on IWildCam results with (a) $w = 10$, $\alpha = 1\%$, and $R = 100$, and (b) $R = 20000$ ⁴. In (a), we bold the best algorithm, and underline the second-best one. In (b), we bold values that exceed the desired $\alpha = 1\%$. For all shifts, our approach achieves the high detection rate ($\geq 80\%$) with the smallest number of samples (Table 4a). All algorithms except DK satisfy the FPR bound (Table 4b).

(a) Number of samples for detection ($\geq 80\%$)			(b) FPR (%) at selected time					
Scn.	Alg.	Natural shift	Scn.	Alg.	300	600	950	1200
M-shift	Ours	670	M-shift	Ours	0.69	0.57	0.68	0.59
	H2	-		H2	0.30	0.35	0.40	0.34
	H5	-		H5	0.46	0.56	0.41	0.45
	Wald	<u>1410</u>		Wald	0.25	0.21	0.26	0.29
	DK	-		DK	1.98	1.91	1.93	1.85
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	4330		ICM	0.18	0.17	0.17	0.22
GI-shift	Ours	3650	GI-shift	Ours	0.66	0.62	0.53	0.57
	H2	-		H2	0.36	0.30	0.40	0.40
	H5	-		H5	0.48	0.51	0.51	0.51
	Wald	<u>4710</u>		Wald	0.17	0.27	0.26	0.29
	DK	-		DK	1.77	1.88	2.10	2.27
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.22	0.17	0.20	0.21
GID-shift	Ours	1620	GID-shift	Ours	0.57	0.59	0.57	0.56
	H2	-		H2	0.33	0.40	0.41	0.36
	H5	-		H5	0.36	0.50	0.51	0.45
	Wald	-		Wald	0.20	0.31	0.25	0.27
	DK	-		DK	1.91	1.82	2.02	2.51
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.24	0.21	0.15	0.19

C.2. Natural shift - Py150

Dataset. All of previous datasets are image datasets. For a more general set-up, we also consider the non-image dataset, Py150 dataset from WILDS dataset. This dataset includes program code from multiple Github repositories, and it has two different test sets: Test (ID) and Test (OOD). The difference between them is that Test (OOD) contains code from different sets of repositories compared to the training set and Test (ID). Similar to IWildCam, a shift from one group of repositories to another group of repositories is considered as a natural shift.

Source-target classifier. We follow the same source-target classifier setting with other natural shift experiments (ImageNet, IWildCam). However, as this dataset is not an image dataset, we use different way of extracting features. We first download

⁴We use $R = 100$ for KDS as it is computationally expensive.

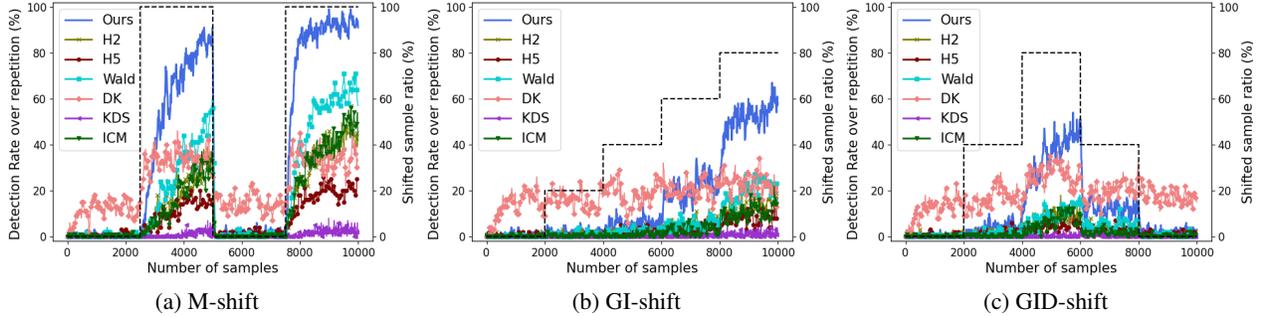


Figure 5: Detection rate for natural shift on Py150 with $R = 100$, $w = 10$, $\alpha = 1\%$. The black dashed line indicates shifted sample ratio, *i.e.*, the degree (or probability) of covariate shift. This shows the similar pattern with IWILDcam experiments (Figure 4). Our approach achieves the high detection rate ($\geq 80\%$) with the smallest number of samples when covariate shift occurs, and it has small FPR when no covariate shift occurs. DK reaches the higher detection rate at the early stage of covariate shift, which may be caused by the higher FPR (Table 4b). DK does not show the notable change in GI-shift case, and we believe that the hyper-parameter was not properly chosen.

Table 5: Natural shift on Py150 results with (a) $w = 10$, $\alpha = 1\%$, and $R = 100$, and (b) $R = 20000$ ⁵. In (a), we bold the best algorithm, and underline the second-best one. In (b), we bold values that exceed the desired $\alpha = 1\%$. For M-shifts, our approach achieves the high detection rate ($\geq 80\%$) with the smallest number of samples (Table 5a), and for the other two shifts, all algorithms cannot reach the high detection rate. All algorithms except DK satisfy the FPR bound (Table 5b). We believe that DK has high FPR because of inappropriate hyper-parameters.

(a) Number of samples for detection ($\geq 80\%$)			(b) FPR (%) at selected time					
Scn.	Alg.	Natural shift	Scn.	Alg.	300	600	950	1200
M-shift	Ours	1570	M-shift	Ours	0.64	0.75	0.84	0.88
	H2	-		H2	0.33	0.40	0.41	0.37
	H5	-		H5	0.49	0.61	0.60	0.63
	Wald	-		Wald	0.24	0.24	0.33	0.41
	DK	-		DK	11.86	13.93	16.90	14.36
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.22	0.22	0.15	0.16
GI-shift	Ours	-	GI-shift	Ours	0.61	0.73	0.76	0.77
	H2	-		H2	0.28	0.31	0.43	0.46
	H5	-		H5	0.45	0.51	0.66	0.83
	Wald	-		Wald	0.18	0.22	0.29	0.34
	DK	-		DK	11.87	13.87	16.98	14.77
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.19	0.18	0.20	0.24
GID-shift	Ours	-	GID-shift	Ours	0.50	0.78	0.85	1.00
	H2	-		H2	0.21	0.37	0.45	0.45
	H5	-		H5	0.41	0.65	0.62	0.73
	Wald	-		Wald	0.18	0.30	0.32	0.38
	DK	-		DK	12.32	14.12	16.83	14.34
	KDS	-		KDS	0.00	0.00	0.00	0.00
	ICM	-		ICM	0.19	0.20	0.21	0.26

the pretrained CodeGPT model (Lu et al., 2021), provided by the authors of WILDS dataset paper (Koh et al., 2021), and run the model and average the embeddings from the model to obtain the final features.

Results. Figure 5 shows the detection rate and Table 5 displays the number of required samples for high detection rate ($\geq 80\%$) and the FPR for the Py150 experiment results.

Discussion. The Py150 results are similar to other experiments with one exception of DK. In M-shift, all algorithms correctly reacts to shift changes. However, in GI-shift and GID-shift, DK does not show notable change in the detection rate even

⁵We use $R = 100$ for KDS as it is computationally expensive.

though sample shift probability changes over time. We believe this is because DK does not have appropriate hyper-parameter for this experiment. In terms of the require number of samples, our algorithm requires the smallest number of samples for M-shift, but all algorithm fail to achieve the high detection rate for GI-shift and GID-shift. All algorithms except DK satisfy the FPR bound, and we believe that the aforementioned DK's hyper-parameter issue results in this high FPR.

C.3. Detection Rate

This section shows the additional detection rate plots for the different perturbations, severities, and window sizes (w) including figures in the main paper.

C.3.1. M-SHIFT

Figure 6 - Figure 15 display the detection rate plot for M-shift scenario with different settings. These all different settings show the similar pattern with the figures in the main paper.

Sequential Covariate Shift Detection

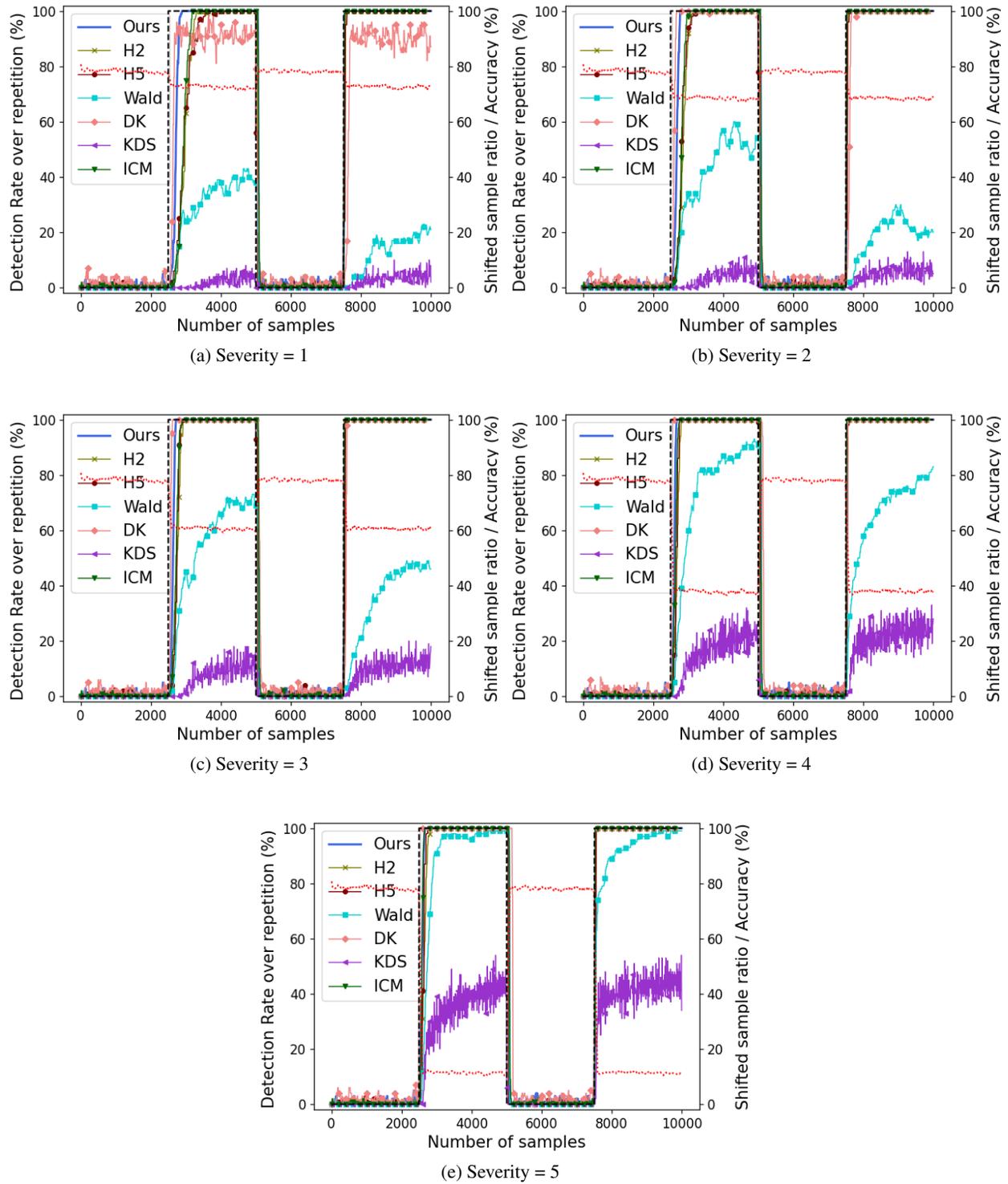


Figure 6: Contrast with $R = 100$, $w = 10$, $\alpha = 1\%$. As the severity increases, all algorithms achieve higher detection rate, and the accuracy of the original classifier drops more. Only DK tends to reach high detection rate with less number of samples when the severity is low. But, DK violates the FPR bound when no covariate shift occurs.

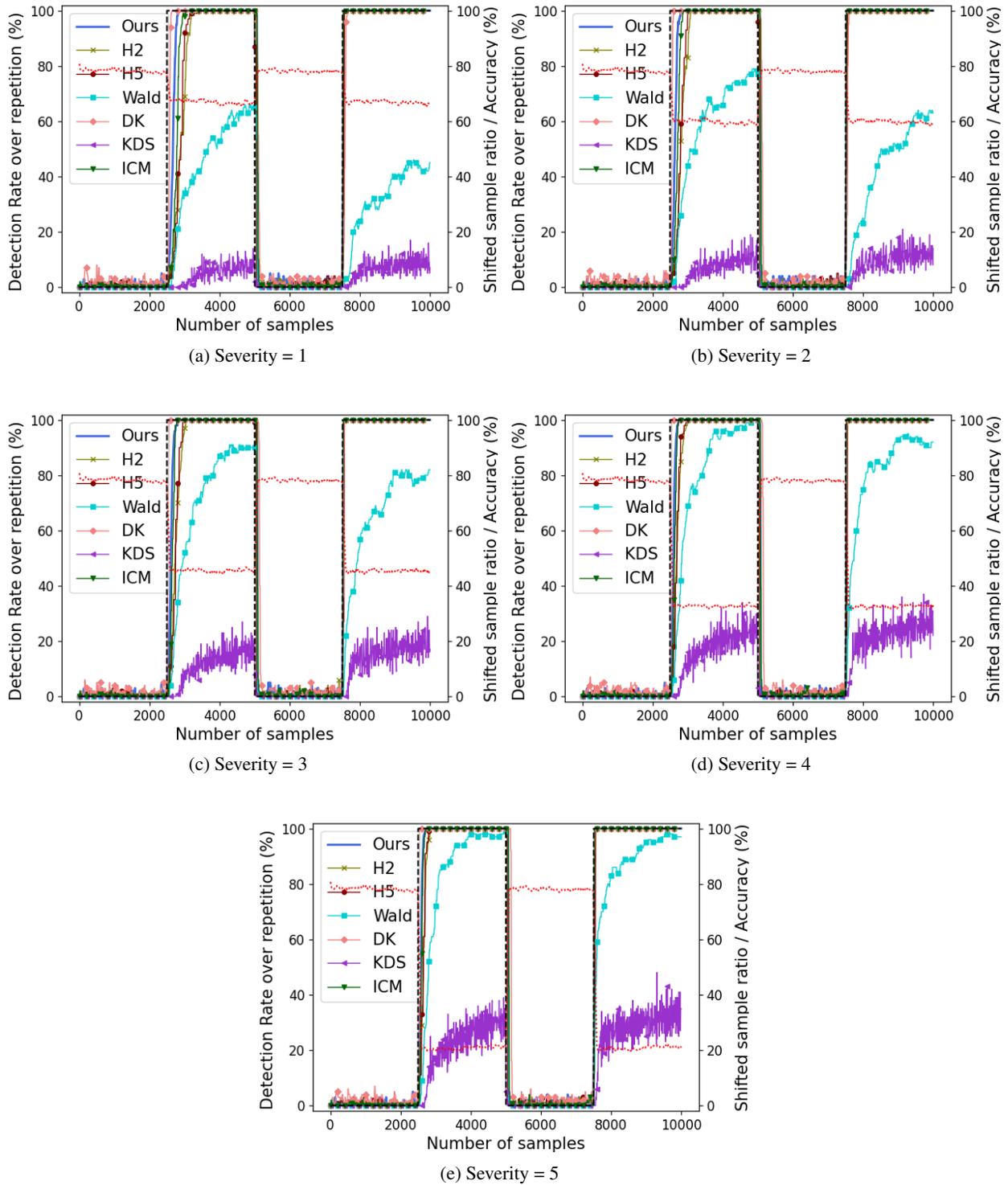


Figure 7: Defocus blur with $R = 100$, $w = 10$, $\alpha = 1\%$. Defocus blur shows the same pattern with Contrast perturbation results (Figure 6).

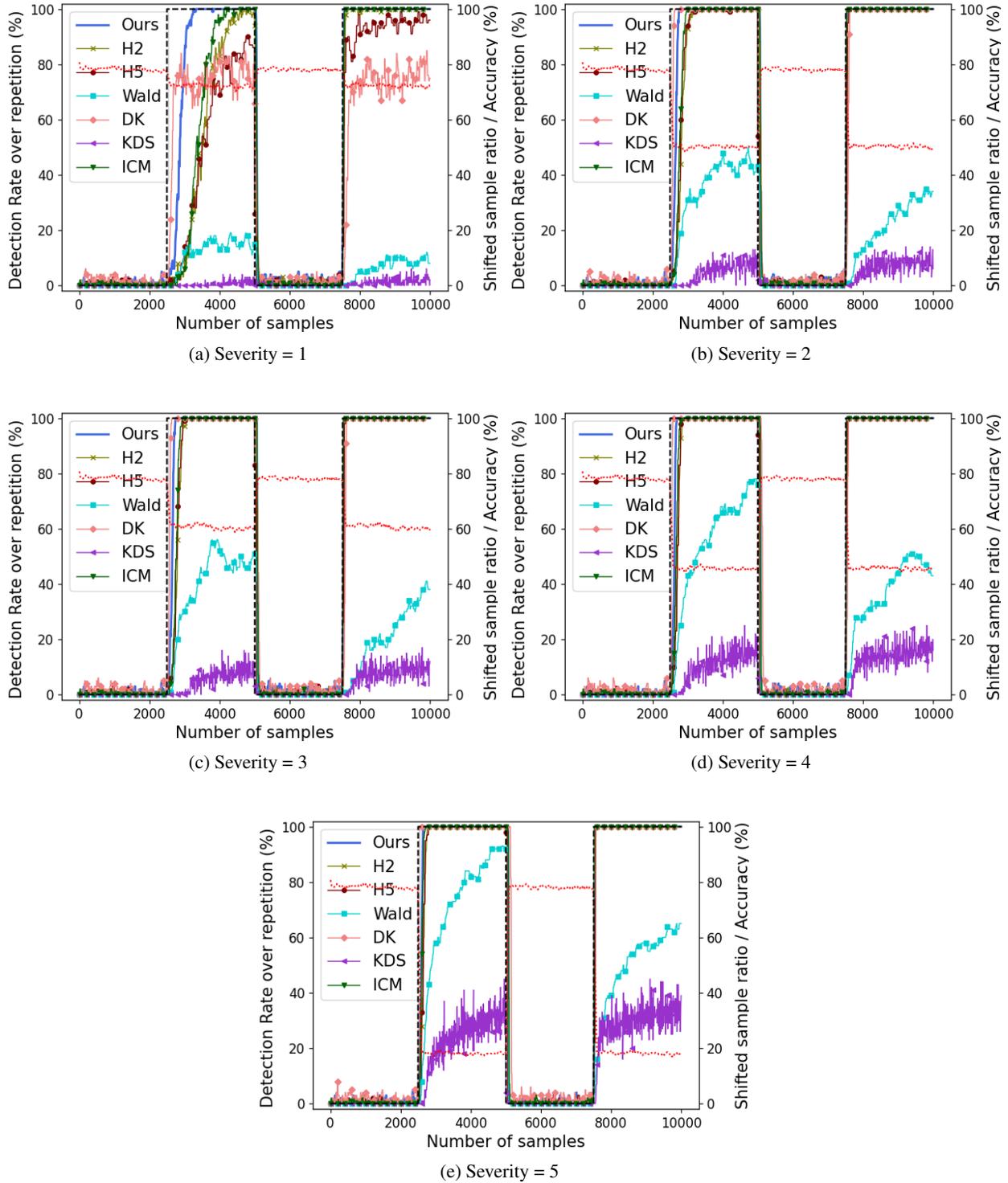


Figure 8: Elastic transform with $R = 100$, $w = 10$, $\alpha = 1\%$. Elastic transform shows the same pattern with Contrast perturbation results (Figure 6).

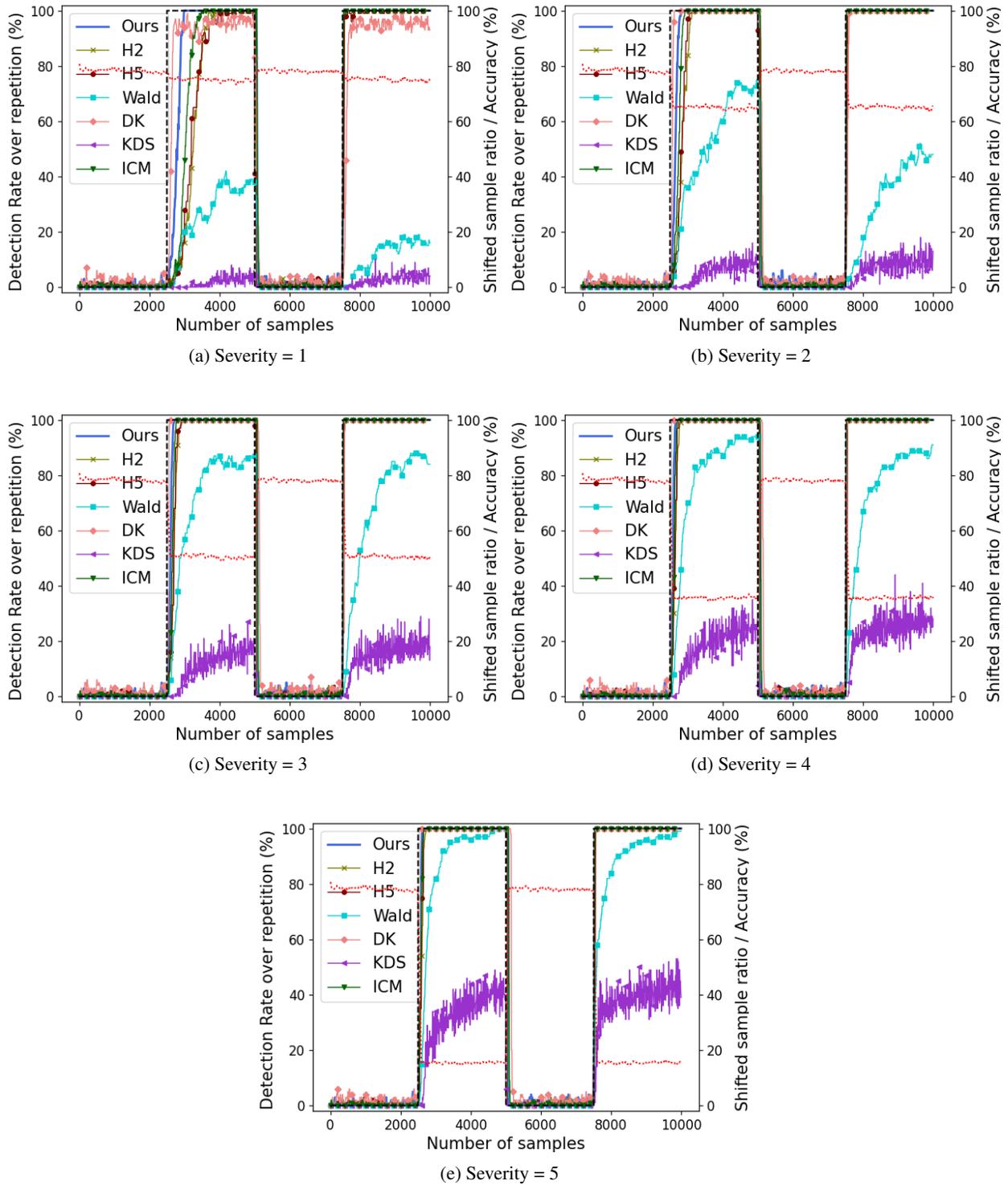


Figure 9: Gaussian blur with $R = 100$, $w = 10$, $\alpha = 1\%$. Gaussian blur shows the same pattern with Contrast perturbation results (Figure 6).

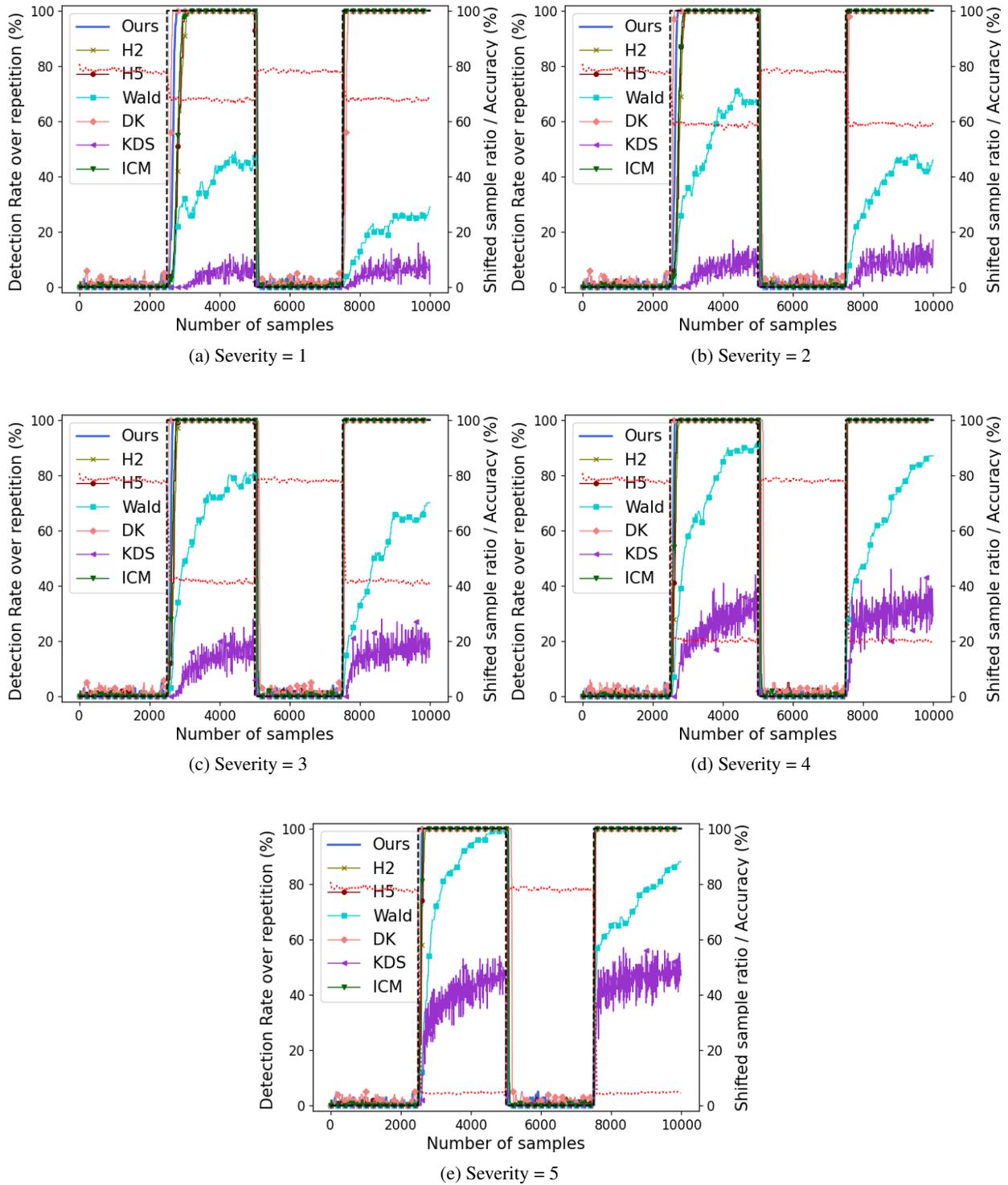


Figure 10: Gaussian noise with $R = 100$, $w = 10$, $\alpha = 1\%$. Gaussian noise shows the same pattern with Contrast perturbation results (Figure 6).

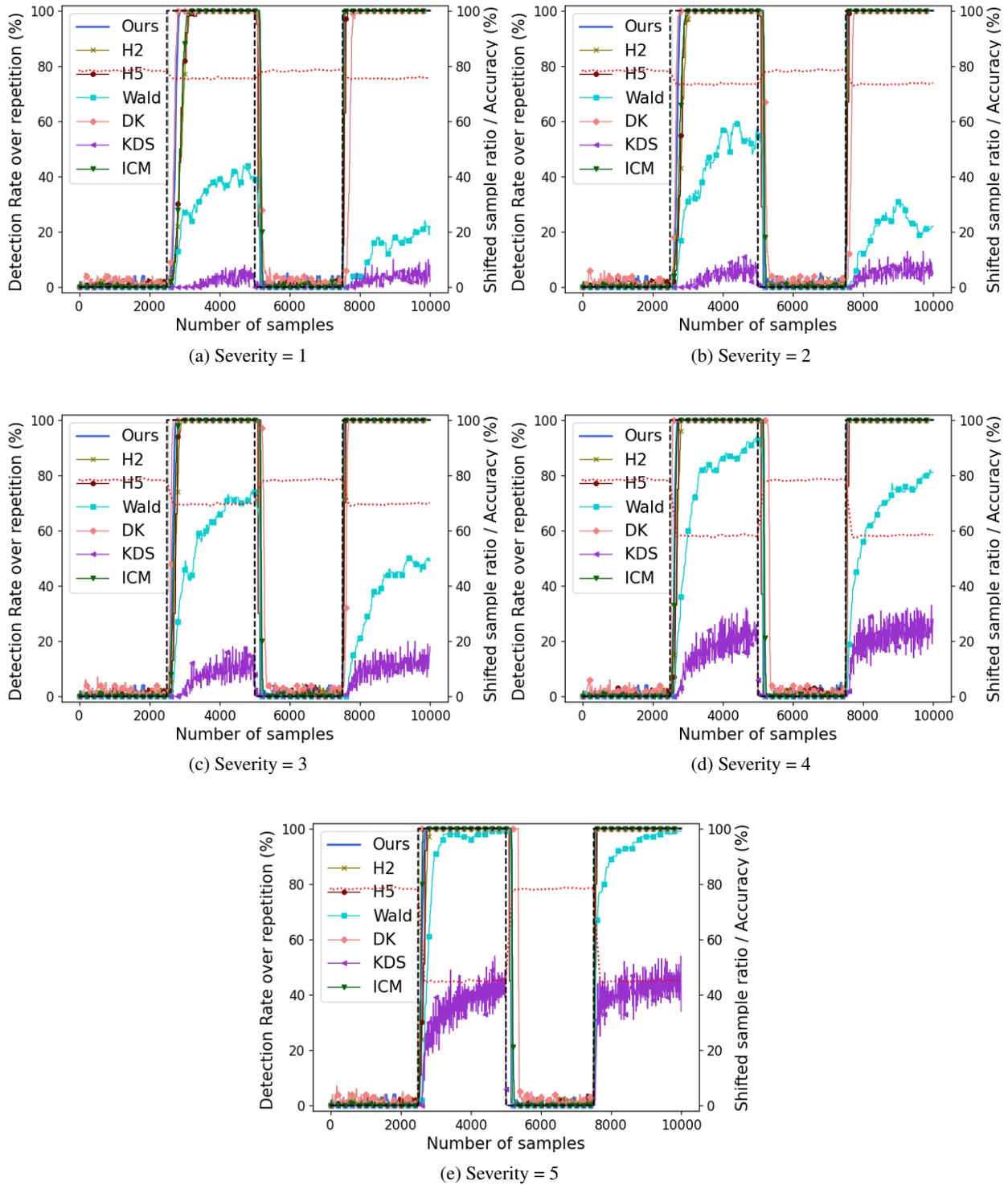


Figure 11: Contrast with $R = 100$, $w = 20$, $\alpha = 1\%$. Compared to $w = 10$ (Figure 6), algorithms detect shifts with less fluctuations, but they show slow reaction to shift change, i.e., near 5000^{th} samples.

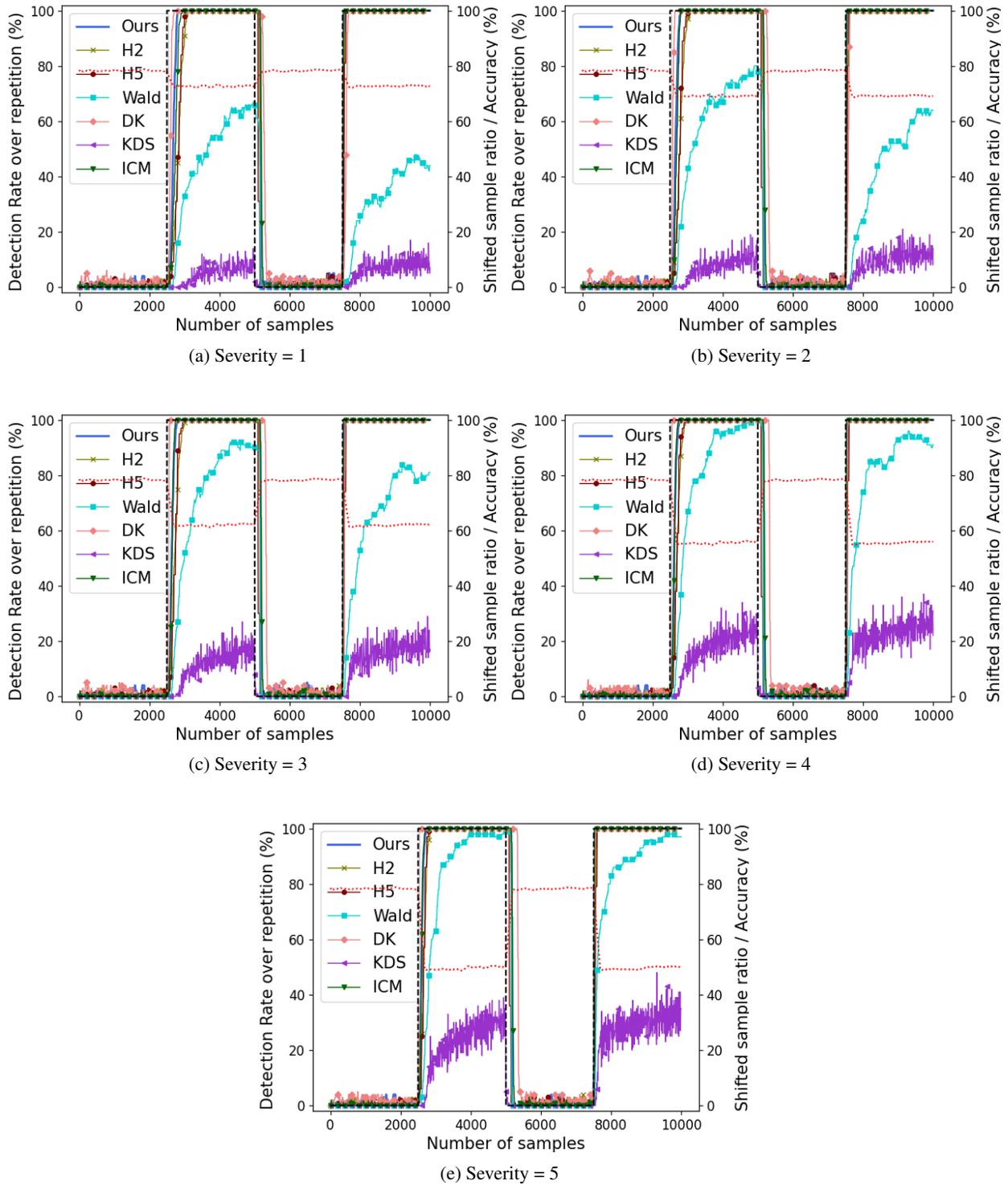


Figure 12: Defocus blur with $R = 100$, $w = 20$, $\alpha = 1\%$. Defocus blur shows similar pattern with Contrast perturbation results (Figure 11).

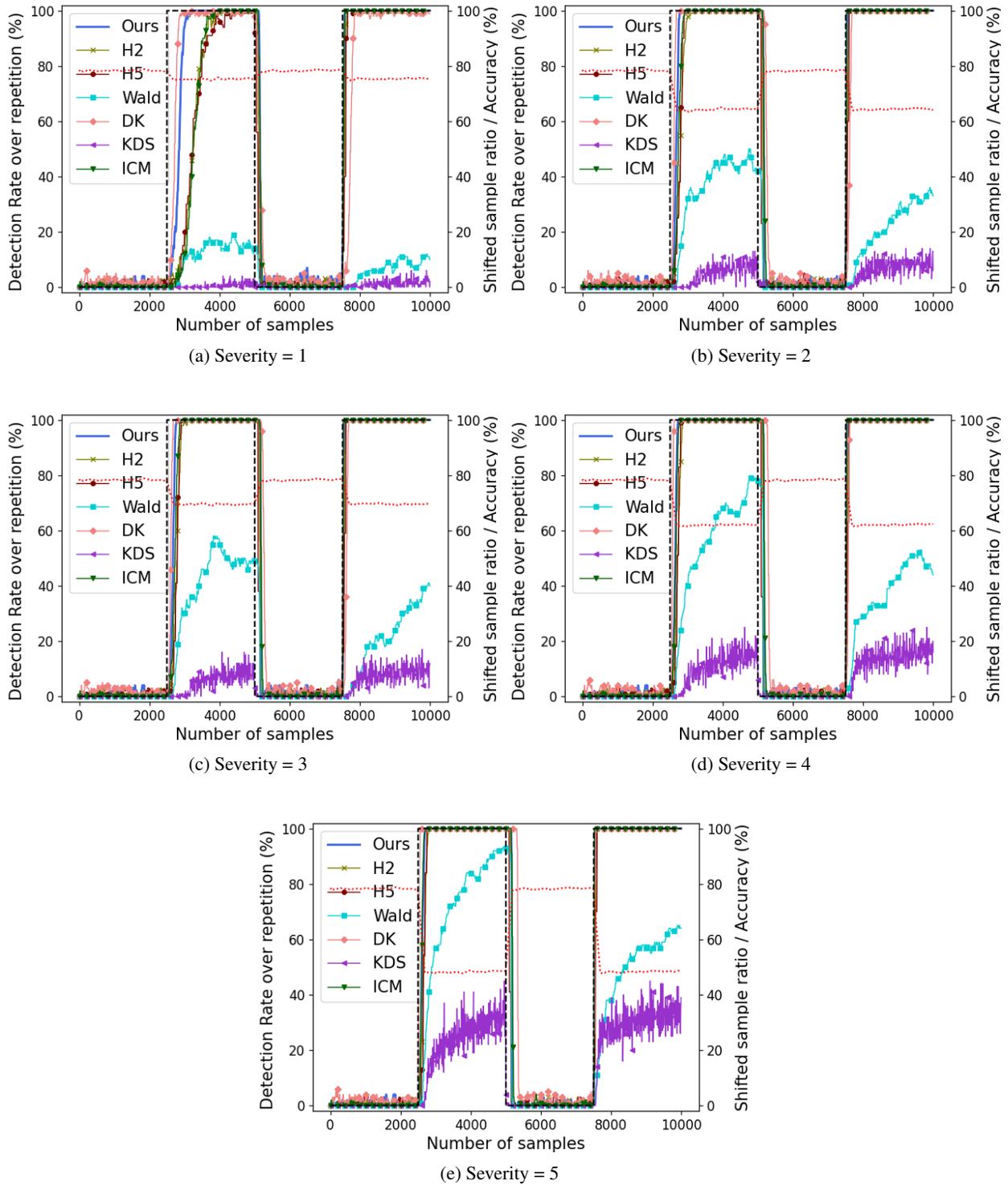


Figure 13: Elastic transform with $R = 100$, $w = 20$, $\alpha = 1\%$. Elastic transform shows similar pattern with Contrast perturbation results (Figure 11).

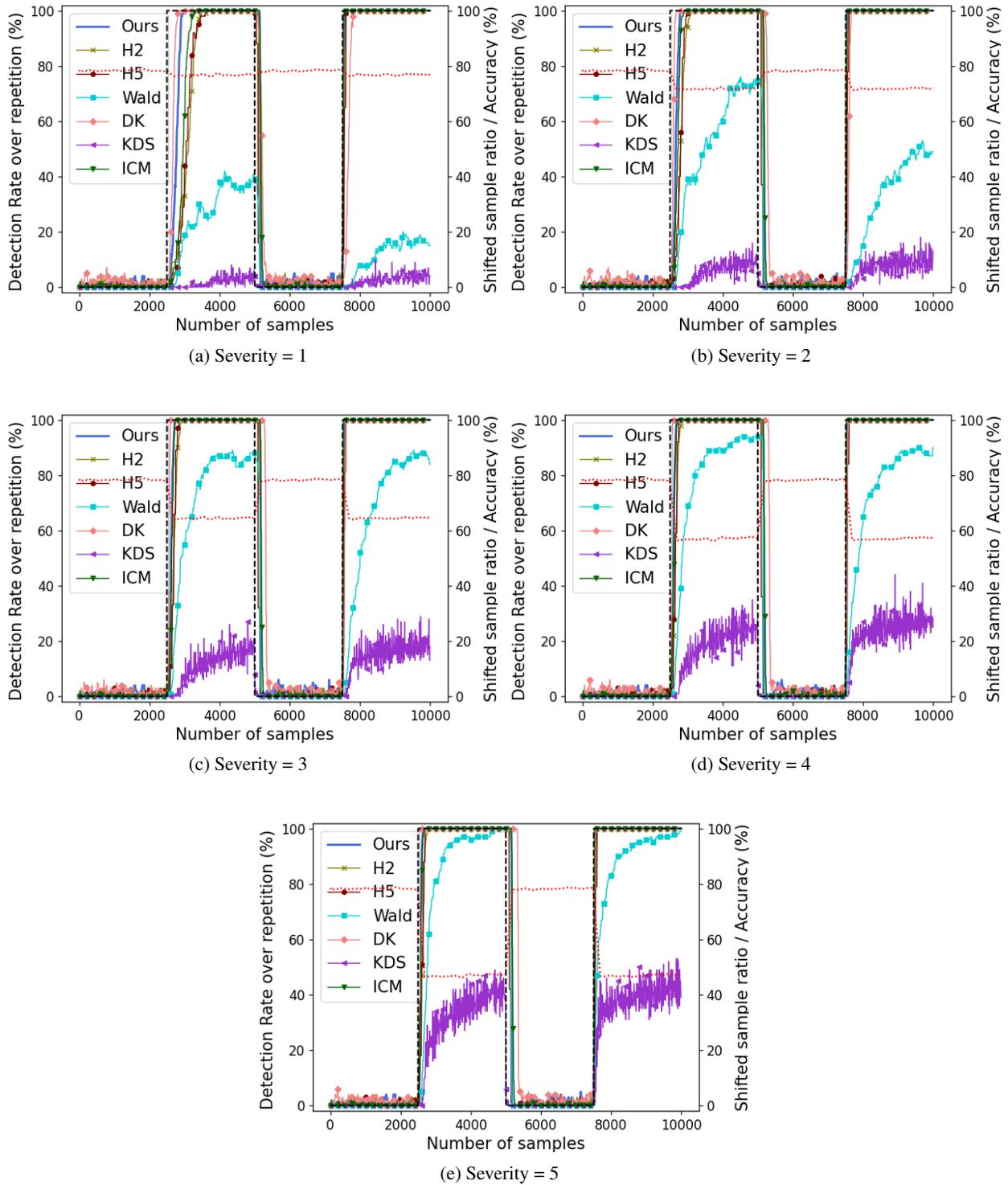


Figure 14: Gaussian blur with $R = 100$, $w = 20$, $\alpha = 1\%$. Gaussian blur shows similar pattern with Contrast perturbation results (Figure 11).

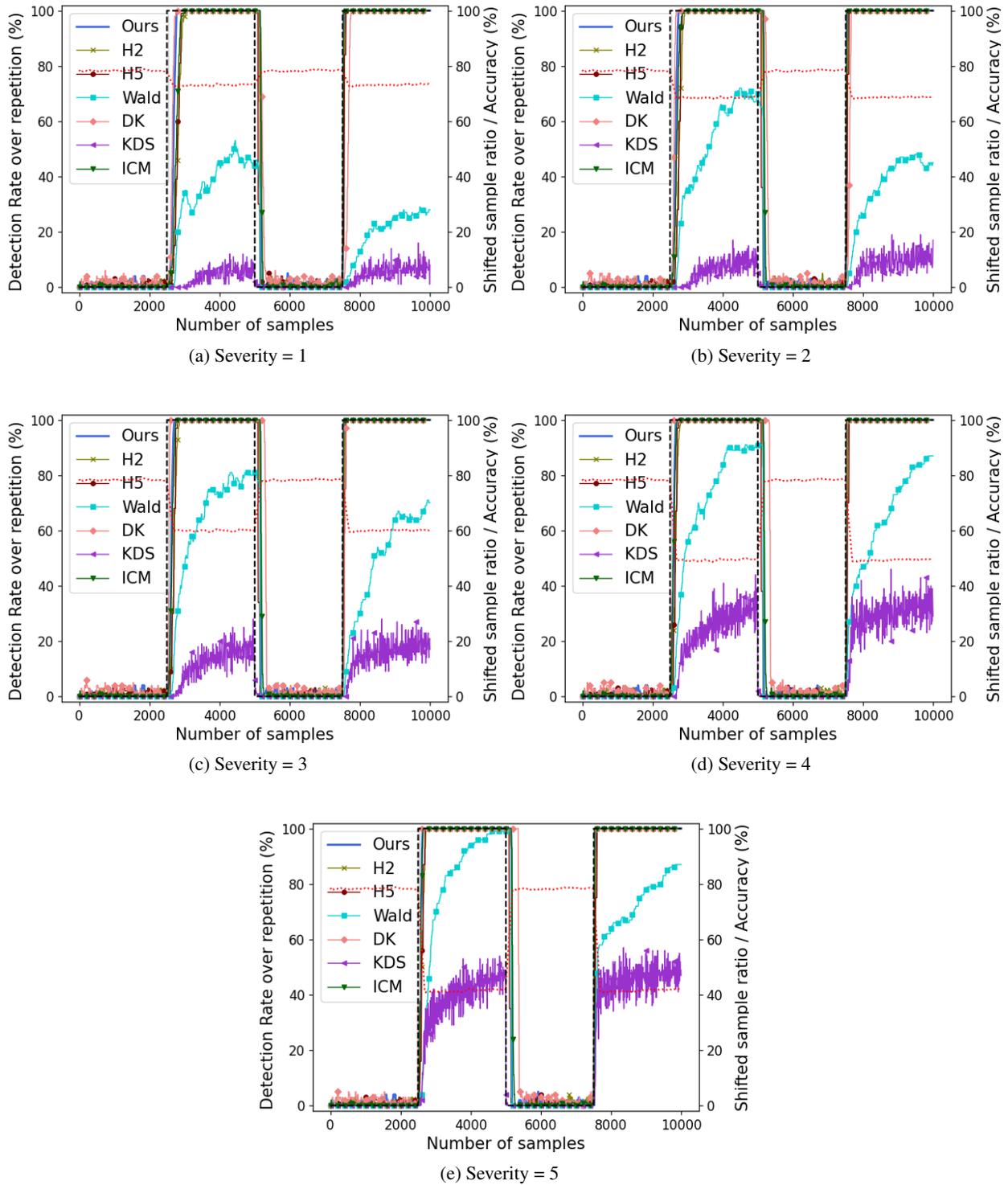


Figure 15: Gaussian noise with $R = 100$, $w = 20$, $\alpha = 1\%$. Gaussian noise shows similar pattern with Contrast perturbation results (Figure 11).

C.3.2. GI-SHIFT

This section includes the plots for GI-shift scenario with different perturbation, window sizes (w), and fixed severity.

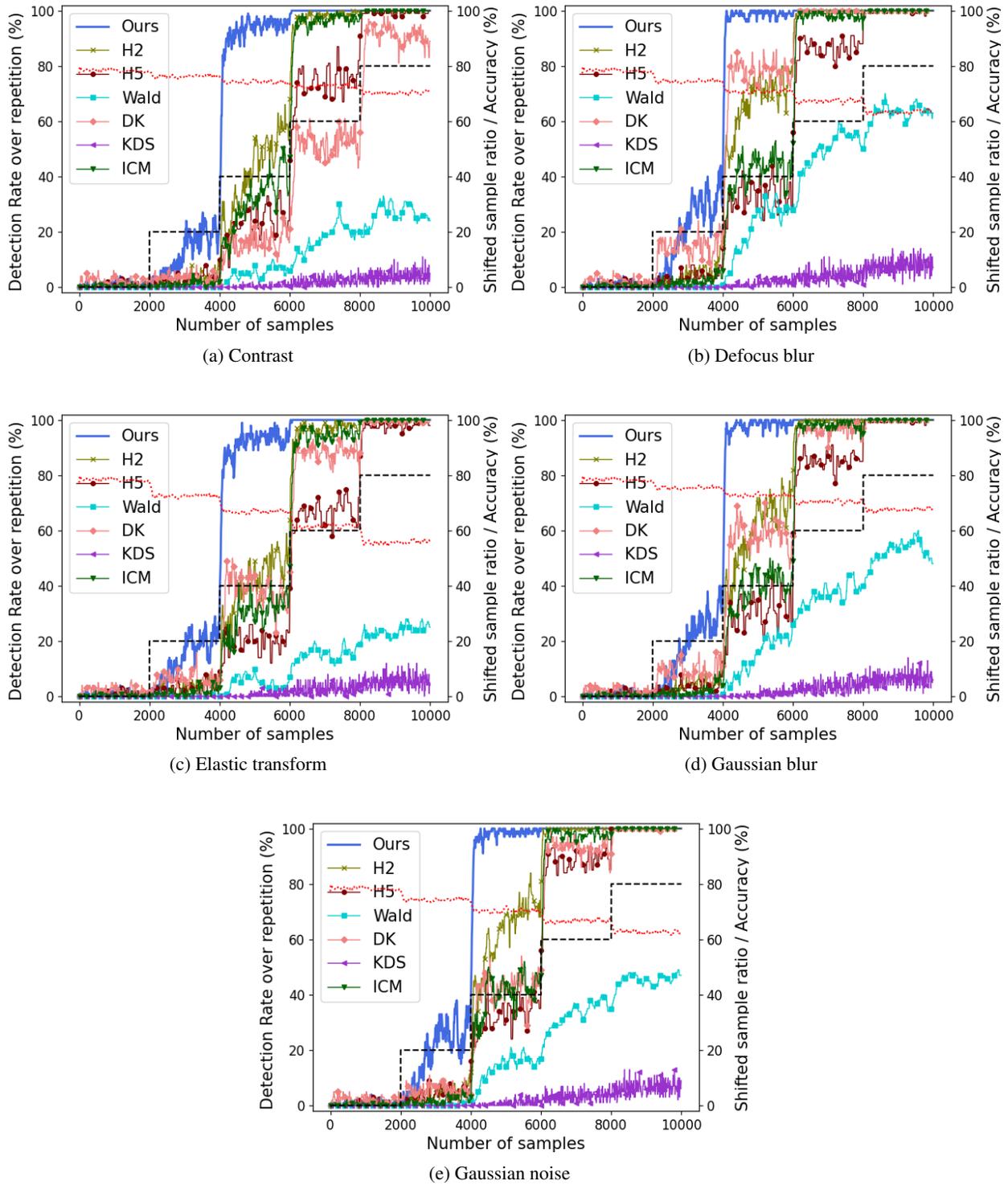


Figure 16: GI-shift with $R = 100$, $w = 10$, $\alpha = 1\%$. All algorithms detect shifts more as the sample shift probability increases. Especially, our algorithm achieves the high detection rate with the shift probability of 40 %.

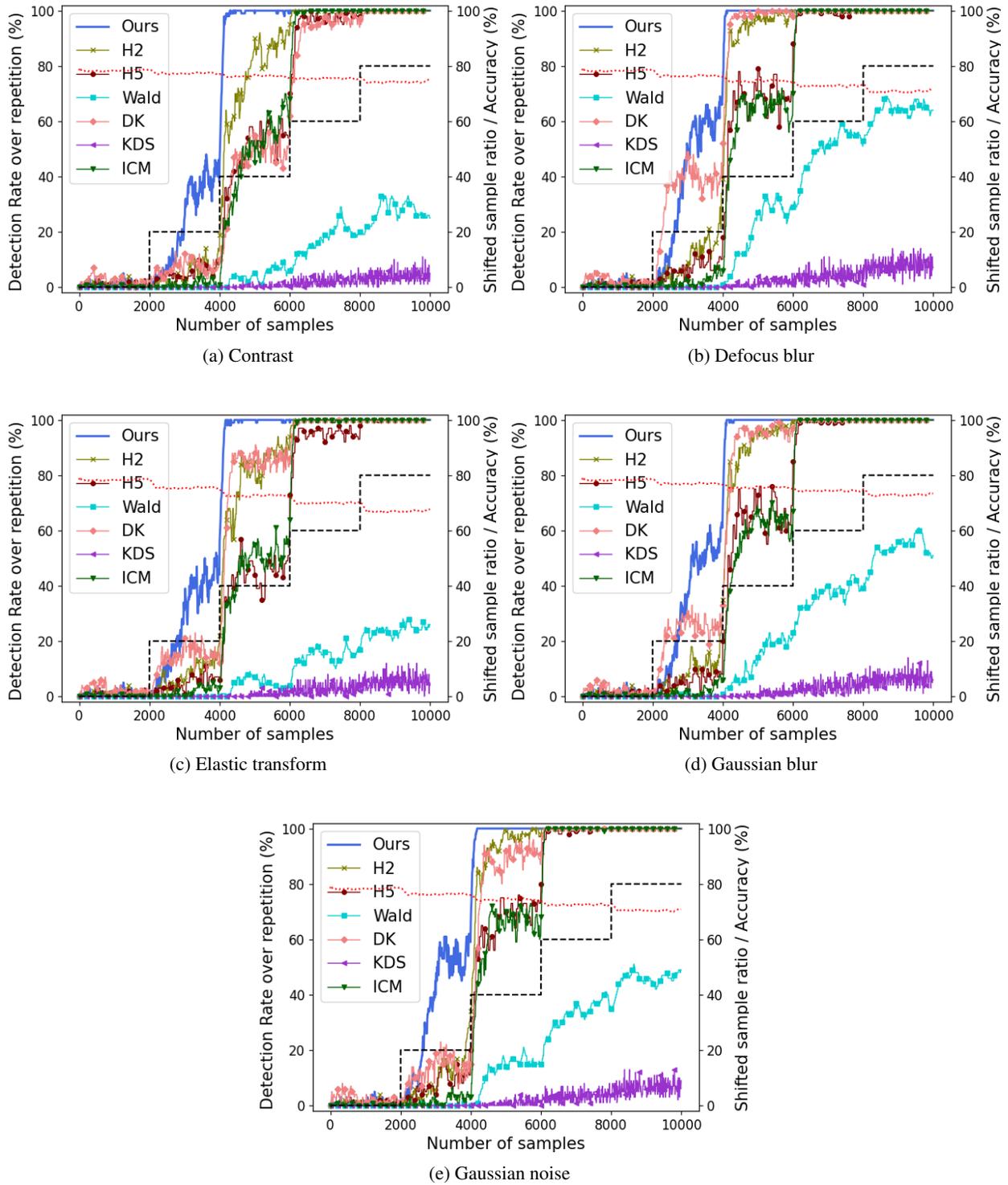


Figure 17: GI-shift with $R = 100$, $w = 20$, $\alpha = 1\%$. Compared to $w = 10$ (Figure 16), all algorithms show less fluctuations in the detection rate.

C.3.3. GID-SHIFT

Similar to the previous two sections, this section includes figures for the GID-shift scenario with different perturbation with severity 2, and different window sizes (w).

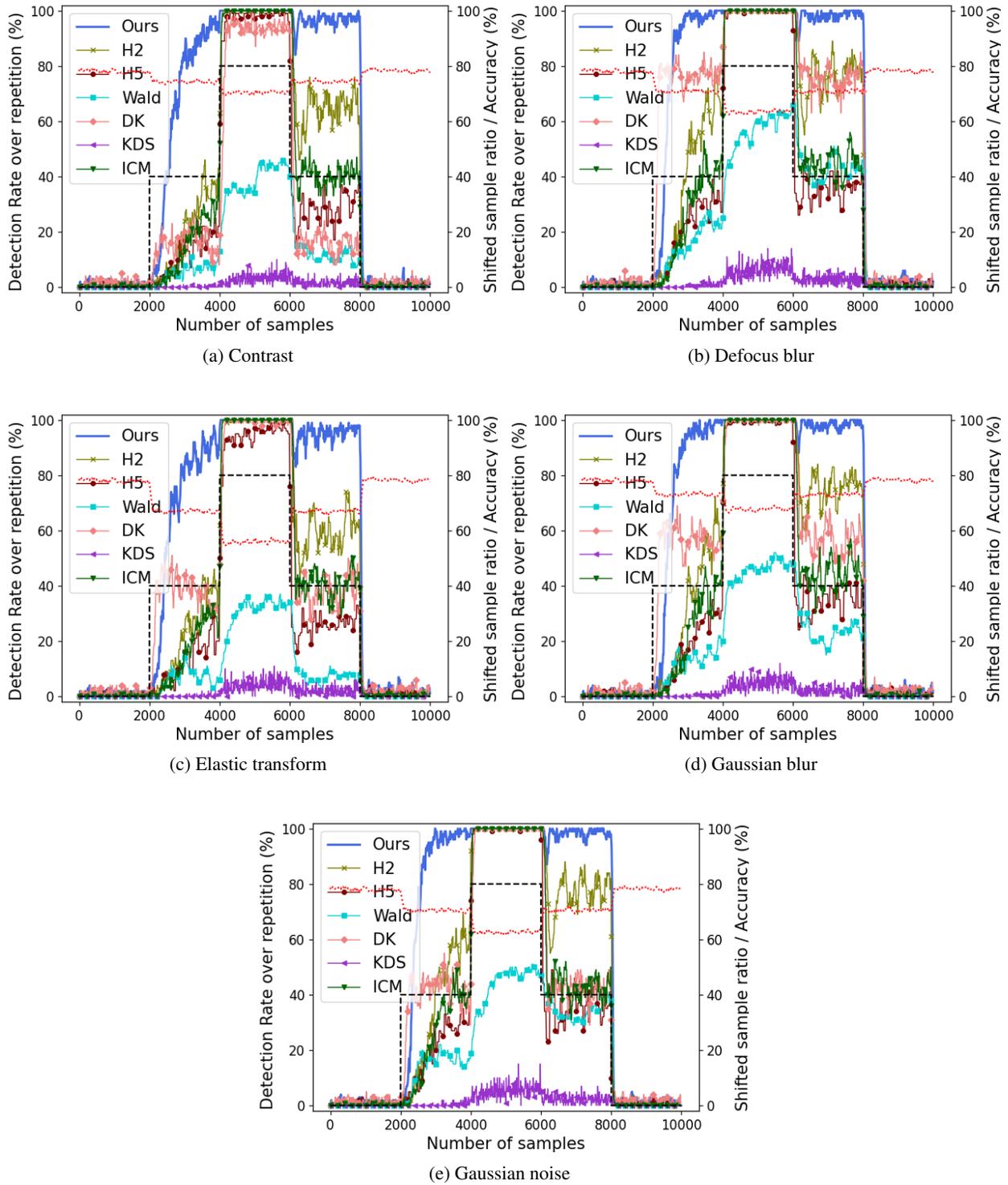


Figure 18: GID-shift with $R = 100$, $w = 10$, $\alpha = 1\%$. All algorithms show the highest detection rate when the sample shift probability is 100 %. But, only our algorithm reaches the high detection rate even when the shift probability is 40 %.

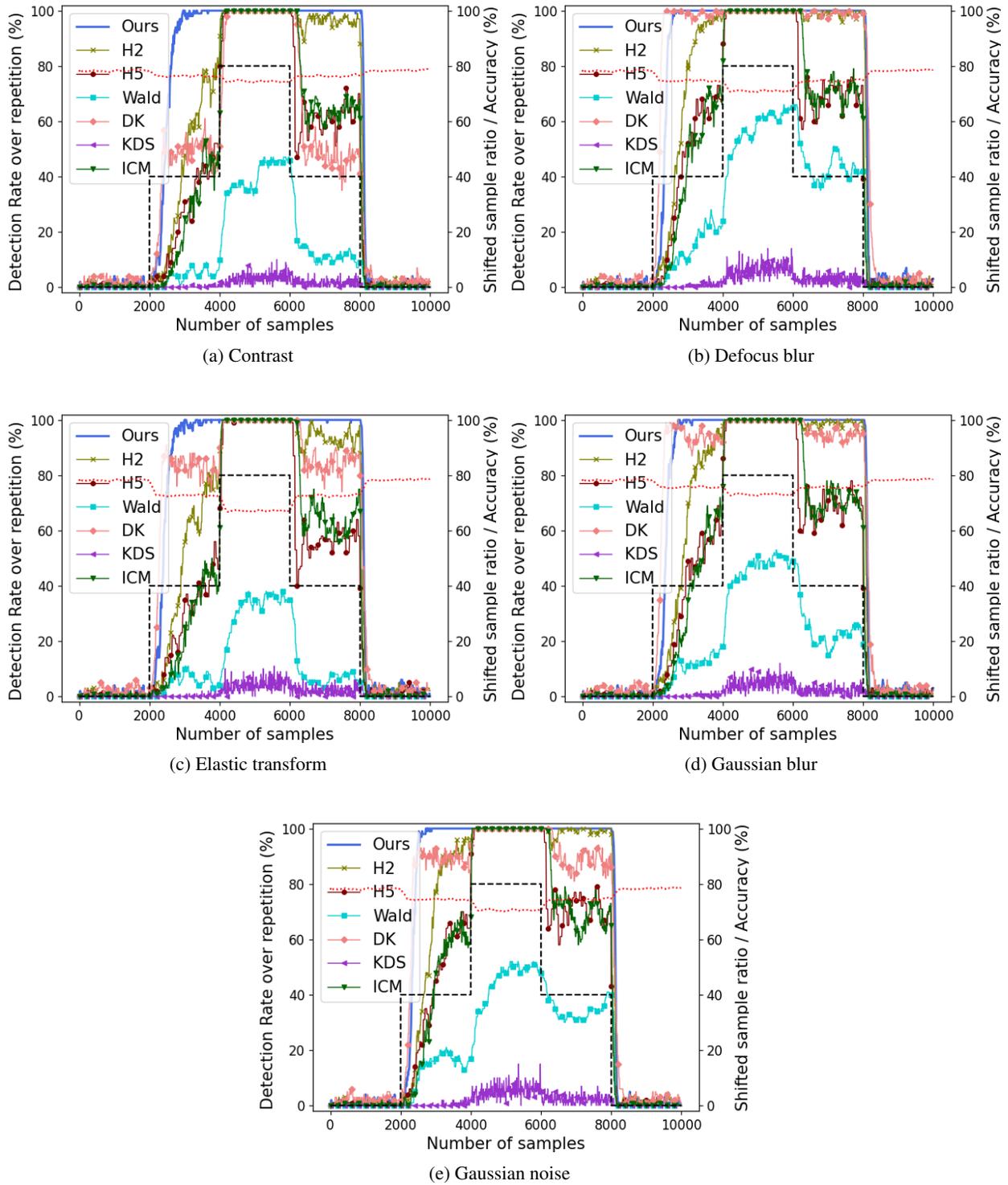


Figure 19: GID-shift with $R = 100$, $w = 20$, $\alpha = 1\%$. Compared to $w = 10$ (Figure 18), all algorithms show the better detection rate with less fluctuations, but, they trigger false positive when the shift disappears, i.e., at 8000th samples.

C.4. Number of Samples for Detection

This section presents the required number of samples for detecting covariate shift over repetitions (Rate $\geq 80\%$) with different perturbations, severities, and window sizes (w).

C.4.1. M-SHIFT

Table 6: Number of samples for detection with $R = 100$, $w = 20$. The bold and underlined numbers means the best and second best results, respectively. DK always requires the smallest number of samples for high detection rate, and our approach shows second-best result except when severity is 5. However, DK violates the FPR bound as shown in the previous experiments.

Severity	Algorithms	Contrast	Defocus Blur	Elastic Transform	Gaussian Blur	Gaussian Noise
1	Ours	<u>300</u>	<u>250</u>	<u>430</u>	<u>360</u>	<u>250</u>
	H2	530	430	970	770	410
	H5	460	410	1010	710	360
	Wald	-	-	-	-	-
	DK	250	150	290	230	190
	KDS	-	-	-	-	-
	ICM	470	330	990	570	350
2	Ours	<u>250</u>	<u>220</u>	<u>240</u>	<u>230</u>	<u>210</u>
	H2	430	390	390	410	350
	H5	360	360	360	360	310
	Wald	-	2410	-	-	-
	DK	190	110	150	130	150
	KDS	-	-	-	-	-
	ICM	350	250	310	290	250
3	Ours	<u>220</u>	200	<u>230</u>	<u>170</u>	<u>170</u>
	H2	330	330	370	290	270
	H5	310	310	360	260	260
	Wald	-	1150	-	990	1770
	DK	150	70	150	90	90
	KDS	-	-	-	-	-
	ICM	270	<u>190</u>	290	190	210
4	Ours	<u>170</u>	<u>170</u>	<u>200</u>	<u>140</u>	<u>140</u>
	H2	270	290	310	230	230
	H5	260	260	260	210	210
	Wald	830	850	-	710	1390
	DK	70	50	110	70	50
	KDS	-	-	-	-	-
	ICM	190	<u>170</u>	210	150	150
5	Ours	160	150	170	110	120
	H2	250	250	230	190	190
	H5	210	210	210	160	160
	Wald	410	610	1330	470	770
	DK	30	50	50	50	30
	KDS	-	-	-	-	-
	ICM	<u>110</u>	<u>130</u>	<u>150</u>	<u>110</u>	<u>110</u>

C.4.2. GI-SHIFT

Table 7: Number of samples for detection with $R = 100$, $w = 20$. The bold and underlined numbers mean the best and second best results, respectively. Our approach always shows the best result while the second best is either H2 or DK.

Algorithms	Contrast	Defocus Blur	Elastic Transform	Gaussian Blur	Gaussian Noise
Ours	2100	2040	2100	2040	2050
H2	<u>2890</u>	2150	2610	<u>2170</u>	<u>2190</u>
H5	4110	4010	4110	4010	4010
Wald	-	-	-	-	-
DK	4150	<u>2130</u>	<u>2310</u>	2230	2310
KDS	-	-	-	-	-
ICM	4050	4050	4050	4050	4050

C.4.3. GID-SHIFT

Table 8: Number of samples for detection with $R = 100$, $w = 20$. The bold and underlined numbers mean the best and second best results, respectively. Mostly, DK shows the best result while our approach comes next. However, DK violates the FPR bound as shown in the previous experiments.

Algorithms	Contrast	Defocus Blur	Elastic Transform	Gaussian Blur	Gaussian Noise
Ours	620	<u>430</u>	<u>530</u>	<u>470</u>	<u>450</u>
H2	1890	990	1670	1170	1030
H5	2010	2010	2060	2010	2010
Wald	-	-	-	-	-
DK	2110	250	370	330	350
KDS	-	-	-	-	-
ICM	2030	2010	2050	2030	2030