Scalable Online Change Detection for High-dimensional Data Streams

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Abstract

Detecting changes in data streams is a core objective in their analysis and has applications in, say, predictive maintenance, fraud detection, and medicine. A principled approach to detect changes is to compare distributions observed within the stream to each other. However, data streams often are high-dimensional, and changes can be complex, e.g., only manifest themselves in higher moments. The streaming setting also imposes heavy memory and computation restrictions. We propose an algorithm, Maximum Mean Discrepancy Adaptive Windowing (MMDAW), which leverages the well-known Maximum Mean Discrepancy (MMD) two-sample test (18), and facilitates its efficient online computation on windows whose size it flexibly adapts. As MMD is sensitive to any change in the underlying distribution, our algorithm is a general-purpose non-parametric change detector that fulfills the requirements imposed by the streaming setting. Our experiments show that MMDAW achieves better detection quality than state-of-the-art competitors.

1 Introduction

Streaming data is generated by a broad variety of sources: sensors in industrial settings, online transactions from financial institutions, click monitoring on websites, twitter feeds, etc. These streams tend to be high-dimensional, i.e., they have many attributes. Quickly detecting when a change takes place in such data is a core objective of its analysis; it allows for, say, predictive maintenance in the industrial setting or for fraud detection when processing transactions.

In general, respective streaming algorithms should fulfill a set of requirements (10; 4): First, each example must be analyzed only once, with low processing time. Second, as the observed stream is potentially unbounded while storage is limited, the storage requirement must be sublinear. Third, one must be able to predict at any time, i.e., detecting changes must happen online.

Assuming that the observed data follows some (unknown) distribution, a change in a stream of data can be defined as a change in the underlying distribution. I.e., there exists a specific point of time, a so-called change point, for which the distributions observable before and after differ (21; 14). A systematic (and widely used) approach to detect whether a change occurred is to employ a statistical test with the null hypothesis that the data from before the potential change point has the same distribution as the data after. If the test rejects the hypothesis, one may assume that a change occurred.

When dealing with real-world data, it is desirable to use non-parametric tests (1). An example of this approach is ADWIN (3), which monitors a stream of data for changes of the mean.

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A well-known statistic to quantify the distance between two arbitrary distributions is Maximum Mean Discrepancy (MMD) (18). It allows to test the hypothesis that two empirical distributions are equal. However, the computation of this statistic has a runtime complexity that is quadratic and requires storage linear in the number of observations, so it does not satisfy the streaming requirements. But unlike other statistics like KL divergence, MMD has the desirable property that its computation does not require an approximation of the probability density function, which is notoriously difficult for high-dimensional data (26; 33; 32).

In this paper, we introduce MMDAW, an algorithm for estimating MMD on data streams, which detects changes in an online fashion. Unlike existing approaches, MMDAW works with multivariate data, is non-parametric, does not have any unintuitive parameters, and can be efficiently computed in the streaming setting. When experimentally comparing MMDAW to competitors, which do not have all these characteristics, we observe a comparable or even superior performance regarding change detection. Specifically, our contributions are the following ones.

We specify a new summary data structure, which slices the data into buckets of exponentially increasing size. At each slice point, the data structure allows computing the value of MMD between data coming before the point to data coming after. We prove that our data structure allows obtaining MMD estimates that are equal to the quadratic time estimates, while reducing the runtime from $O(t^3)$ to $O(t \log t)$ per insert, for a stream of length $t$. The structure has just one parameter, the basis of the geometric law to use, which is intuitive and allows trading off runtime for result quality.

We propose MMDAW, a new, general change detection algorithm. It leverages the above data structure and improves the runtime using a logarithmic sampling scheme, reducing the memory complexity from $O(t)$ to $O(\log t)$. While this slightly impairs the quality of the estimate, it facilitates its efficient computation. We generalize the MMD two-sample test to sets of different sizes to then detect changes with a runtime complexity of $O(\log^2 t)$ for each new data point, i.e., runtime and memory complexity are sublinear. MMDAW fulfills the aforementioned requirements and has the level of the statistical test as its only additional parameter.

We analyze our algorithm. We derive the number of terms it uses for estimating MMD. The result implies that the combination of our data structure with subsampling improves the estimate compared to subsampling in isolation.

We run extensive experiments on standard benchmark data. They reveal that our algorithm performs better than state-of-the-art approaches on all five tested data sets when considering larger detection delays and better on three when considering smaller delays, using the $F_1$-score.

We release our source code on GitHub, together with our experiments, to ensure reproducibility.

2 Related Work

In contrast to drift detection, change detection is unsupervised in nature (14): Given a stream of data, the task is to identify changes in the underlying distribution. The problem has received and still is receiving considerable attention. One can classify existing approaches as parametric and non-parametric. As parametric methods tend to rely on specific assumptions, they often are not applicable to real-world scenarios (1), so we limit our review to non-parametric approaches.

A natural way to detect a change point in data is to use a statistical test. ADWIN (3) is the classic example, but it is limited to univariate data and only detects changes in the mean of the data observed. Addressing the former, (12) introduce ADWINK, an ensemble of ADWIN instances of which a fixed number must agree on whether a change occurred. They find that this ensemble of univariate change detectors often outperforms multivariate detectors. The existing approach conceptually most similar to ours is by Dasu et al. (6). However, they estimate the density of the data as a preliminary step. This does not readily scale to a large number of dimensions (26; 33; 32). Indeed, many change detection algorithms tend to perform well on univariate data and on low-dimensional multivariate data (20), but their detection quality drops as the number of dimensions increases (11).

In our experiments, we compare MMDAW to ADWINK, IBDD (7), WATCH (11), and D3 (16). They all explicitly target at change detection in high-dimensional data. The idea behind IBDD is to generate a reference image from the start of the stream and of new data and to continuously compare
both of them. A change is flagged if both are significantly different. Like MMDAW, WATCH employs hypothesis testing but relies on Wasserstein distance instead. D3 uses a different approach: It maintains two sliding windows of the data stream, and trains a classifier to distinguish their elements, flagging a change if the classifier performance, measured by AUC, exceeds a threshold. But relying on a separate classifier increases the number of parameters, complicating the configuration.

Our algorithm relies on a two-sample test [13] employing kernel mean embeddings [27] and on summary statistics [36] to approximate MMD. [13] introduce a linear time statistic that estimates MMD on data streams. However, its statistical power is relatively low, and its generalization for online change detection is not straightforward. Addressing the former, [35] introduce $B$-tests to improve the statistical power. See [24] for an overview of kernel mean embeddings.

There exist approaches deploying kernel methods for change detection. [9] for instance use an SVM-based approach to detect abrupt changes in streams. The change detection method of [19] also builds on a hypothesis test and, although it relies on a different test statistic, it is in principle similar to ours. However, their algorithm has cubic complexity, so it does not fulfill the streaming requirements.

3 Maximum Mean Discrepancy Adaptive Windowing

3.1 Background and Notation

**Problem definition.** We are given a stream of data, i.e., a possibly infinite sequence of observations $x_1, x_2, \ldots, x_t, \ldots$ for $t = 1, 2, \ldots$ and $x_t \in X$, where $X$ is an arbitrary set. Each $x_t$ is generated independently following some distribution $D_t$. If there exists $k$ such that for $i < k$ and $j \geq k$ we have that $D_i \neq D_j$, the algorithm must detect $k$, i.e., the time at which a change occurred, while fulfilling the requirements laid out in the introduction.

**Kernel mean embedding.** Let $\mathcal{H}$ be a Reproducing Kernel Hilbert Space (RKHS) on a set $X$, i.e., for $x \in X$ the linear evaluation functional $\delta_x : \mathcal{H} \rightarrow \mathbb{R}$ defined by $\delta_x(f) = f(x)$ is bounded [24]. By the Riesz representation theorem [25], there exists for each $x \in X$ a unique vector $\Phi(x) \in \mathcal{H}$ such that for every $f \in \mathcal{H}$, $f(x) = \delta_x(f) = (f, \Phi(x))$. The function $\Phi(x)$ is the reproducing kernel for $x$ and also called feature mapping, it has the canonical form $\Phi(x) = k(x, \cdot)$ [28]. The function $k : X \times X \rightarrow \mathbb{R}$ is the reproducing kernel for $\mathcal{H}$ [24]. Note that we have $k(x_1, x_2) = (\Phi(x_1), \Phi(x_2))$.

Next, we define the embedding of a probability distribution. Let $p$ be a Borel probability measure. The mean embedding of $p$ is defined as the element $\mu_p \in \mathcal{H}$ such that $\mathbb{E}_x f = (f, \mu_p)$ for all $f \in \mathcal{H}$. The mean embedding $\mu_p$ exists if $k(\cdot, \cdot)$ is measurable and $\mathbb{E}_{x \sim p} \sqrt{k(x,x)} < \infty$ [13, 27, 18].

**Maximum mean discrepancy.** Following [18], let $\mathcal{F}$ be a class of functions $f : X \rightarrow \mathbb{R}$, and let $x, y$ be random variables on a topological space $X$ with Borel probability measures $p, q$. We abbreviate $\mathbb{E}_{x \sim p} \cdot$ by $\mathbb{E}_x \cdot$, and $\mathbb{E}_{y \sim q} \cdot$ by $\mathbb{E}_y \cdot$, where $x \sim p$ means that $x$ has distribution $p$. Maximum Mean Discrepancy is then defined as $\text{MMD}^2[\mathcal{F}, p, q] = \sup_{f \in \mathcal{F}} \mathbb{E}_x [f(x)] - \mathbb{E}_y [f(y)]$.

By [18] Lemma 4, we have that $\text{MMD}^2[\mathcal{F}, p, q] = \|\mu_p - \mu_q\|^2$, assuming that the mean embeddings $\mu_p, \mu_q$ exist. Further, if $\mathcal{F}$ is a unit ball in an universal RKHS $\mathcal{H}$ defined on a compact metric space $X$, then MMD is a metric. See [18] for technical details.

**MMD estimation.** Following [18] Lemma 6, let $x, x'$ be independent random variables with distribution $p$, and let $y, y'$ be independent random variables with distribution $q$. The squared population MMD in terms of kernel functions then is

$$\text{MMD}^2[\mathcal{F}, p, q] = \mathbb{E}_{x,x'}[k(x,x')] - 2 \mathbb{E}_{x,y}[k(x,y)] + \mathbb{E}_{y,y'}[k(y,y')].$$

For observations $X = \{x_1, \ldots, x_m\}, Y = \{y_1, \ldots, y_n\}$, a biased sample estimate is given by

$$\text{MMD}_b^2[\mathcal{F}, X, Y] = \frac{1}{m^2} \sum_{i,j=1}^m k(x_i, x_j) + \frac{1}{n^2} \sum_{i,j=1}^n k(y_i, y_j) - \frac{2}{mn} \sum_{i=1}^m \sum_{j=1}^n k(x_i, y_j).$$

We take MMD$^2$ as gold standard for the estimate of MMD obtained by MMDAW.
Hypothesis testing. We need our algorithm to answer the question whether the value of MMD indicates that the distributions of sets of data $X \sim p$ and $Y \sim q$ are statistically significantly different, i.e., we test the null hypothesis $H_0 : p = q$ versus its alternative $H_1 : p \neq q$. To this end, we compare the test statistic to a particular threshold $\epsilon_\alpha$. We fail to reject the hypothesis if the value of the test statistic is below this threshold; we reject it otherwise. $\alpha$ is the level of the test, and a bound for the probability that it rejects $H_0$ incorrectly (5). (13) provides the threshold $\epsilon_\alpha$ for MMD$^2$ in the case that $m = n$, i.e., both samples have the same size. This generally does not hold in our case: In a data stream, there usually is a different number of observations from before and after a change point, i.e., $m \neq n$. So we generalize their result in the following.

3.2 MMDAW Data Structure and Algorithm

The naive solution to detect a change in the distribution of the data $W$ observed until time $t$ is storing all data and, for every possible split into two neighboring windows $W = X \cdot Y$, testing the hypothesis $H_0 : \text{“The distributions in } X \text{ and } Y \text{ are equal”, i.e., checking whether } \text{MMD}^2[\mathcal{F}, X, Y] < \epsilon_\alpha$. As the computation of Equation (3) is in $O(t^2)$, and we compute the equation $t$ times, the naive solution has a runtime complexity of $O(t^3)$ per insert operation and a memory requirement of $O(t)$, assuming that the computation of $\epsilon_\alpha$ is $O(1)$.

To reduce the runtime complexity, we first propose a data structure which slices the data into buckets whose size increases over time according to a geometric law (3). Our contribution here is an incremental update scheme that allows to obtain the precise value of MMD$^2$ between neighboring buckets. To reduce the memory complexity, we then propose to subsample within our data structure.

In concrete terms, to simplify exposition, we first fix a basis $b$ for the geometric law to use. This allows trading off runtime for granularity and, w.l.o.g., we set $b = 2$ for all that follows, corresponding to the most fine-granular setting. After observing $t$ elements, the number of buckets corresponds to the number of ones in the binary representation of $t$. We may thus index the buckets $B_1, \ldots, B_b$, with position $l = 0, \ldots, \lfloor \log_2 t \rfloor$, and a bucket must not necessarily exist. In our data structure, a bucket $B_t$ at position $l$ stores $2^l$ observations $x_1, \ldots, x_{2^l}$. Further, $B_t$ stores the sum $XX_t = \sum_{i,j=1}^{2^l} k(x_i, x_j)$ of the kernel evaluated on all pairs of its observations, and a list of sums $XY_t = \left\{ \sum_{i=1}^{2^l} \sum_{j=1}^{2^l} k(x_i, x_j^{l+1}), \ldots, \sum_{i=1}^{2^l} \sum_{j=1}^{2^l} k(x_i^{l+1}, x_j^{l+1}) \right\}$ of the kernel evaluated on pairs of its own observations and the observations in buckets coming before it. The length of $XY_t$ equals the number of buckets having observations older than bucket $B_t$ and is at most $\lfloor \log_2 t \rfloor$.

The following proposition establishes that we can precisely compute MMD$^2$ between buckets.

**Proposition 1.** Given a list of neighboring buckets $B_{k}, \ldots, B_{s+1}, B_{s}, \ldots, B_{l}$ and a position $s, k > s > l$, let $X = x_1, \ldots, x_m$ be the observations in buckets $B_k, \ldots, B_{s+1}$, and let $Y = y_1, \ldots, y_n$ be the observations in buckets $B_{s}, \ldots, B_l$. We can then compute $\text{MMD}^2[\mathcal{F}, X, Y]$ with a runtime complexity logarithmic in the number of observations.

**Proof.** First, note that given two buckets $B_i, B_j$, we may trivially compute MMD$^2$ of their respective observations $X, Y$ with

$$\text{MMD}^2[\mathcal{F}, X, Y] = \frac{1}{m^2} XX_i + \frac{1}{n^2} XX_j - \frac{2}{mn} XY_{ij},$$

where $XX_i, XX_j$, and $XY_{ij}$ are already stored within buckets $B_i, B_j$, i.e., the complexity is $O(1)$. We will now show that by using the above structure, we may efficiently merge two buckets $B_i, B_j$ of size $m, n$ with observations $x_1, \ldots, x_m$ of $B_i$, and $y_1, \ldots, y_n$ of $B_j$, to obtain the correct values for $XX$ and $XY$ of the new bucket. The general result then follows by induction.

Let $B'$ be the new bucket we create and define $x_{m+1}, \ldots, x_{m+n} := y_1, \ldots, y_n$. Clearly, $B'$ must store $XX = \sum_{i,j=1}^{m+n} k(x_i, x_j)$ and a list $XY$ corresponding to the buckets coming before it. To compute $XX$, note that by Iverson’s convention (17), we have for all natural numbers $i, j$ that $[1 \leq i, j \leq m + n] = [1 \leq i, j \leq m] + [m + 1 \leq i, j \leq m + n] + [1 \leq i \leq m, m + 1 \leq j \leq m + n] + [1 \leq j \leq m, m + 1 \leq i \leq m + n]$. Hence, we may decompose the sum for a symmetric
With the data structure and the computation of MMD established, we propose Algorithm 1 for change detection on data streams: It starts with an empty list of buckets. Then, for each new observation, it subsamples a logarithmic number of observations in the list of buckets coming before it. The same holds for \( B_t \) for which the list has one more element \((XY_0^1)\) used above. As the elements in \( XY \) are additive, it suffices to merge both lists by adding their values element-wise, omitting \( XY_0^1 \), and storing the result in \( B' \). As each list has at most \( \log t \) elements, merging them is \( O(\log t) \), and this concludes the proof.

With the data structure and the computation of MMD established, we propose Algorithm 1 for change detection on data streams. The following proposition and its corollary give the value for threshold \( \epsilon \).

**Proposition 2.** Let \( p, q, X, Y \) be defined as before, and assume \( 0 \leq k(x, y) \leq K \), and \( p = q \). Then

\[
P\{MMD_0(F, X, Y) - (K/m + K/n)^{1/2} \geq \epsilon\} \leq \exp \left( -\frac{t^2 mn}{2K(m+n)} \right) .
\]

**Proof.** The proof follows [18, Proof A.3] without assuming \( m = n \), see our Appendix A.2. \( \square \)

**Corollary 1.** A hypothesis test of level \( \alpha \) for \( p = q \) has acceptance region

\[
MMD_t(F, X, Y) < \sqrt{\frac{K}{m} + \frac{K}{n}} \left( 1 + \sqrt{2\ln \alpha^{-1}} \right) .
\]

**Proof.** Set \( \alpha = \exp \left( -\frac{t^2 mn}{2K(m+n)} \right) \) and solve for \( t \) to obtain a test of level \( \alpha \). \( \square \)

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**Algorithm 1 MMD with Adaptive Windowing (MMDAW)**

**Require:** Data stream \( x_1, x_2, \ldots \), level \( \alpha \)

**Output:** Change points in \( x_1, x_2, \ldots \) and times at which change points were detected

1: \( \text{buckets} \leftarrow \emptyset \)
2: \( \text{for each } x_i \in \{x_1, x_2, \ldots \} \) do
3: \( \text{XX}_0 \leftarrow k(x_i, x_i) \quad \triangleright \text{Initialize } B_0 \)
4: \( \text{for each } B_j \in \text{buckets} \) do
5: \( \text{XY}_0^1 \leftarrow \sum_{i=1}^{\lvert B_j \rvert} k(x_i, x_i) \)
6: \( \text{buckets} \leftarrow \text{buckets} \cup B_0 \)
7: \( \text{for every split } s \text{ in } \text{buckets} = \{B_k, \ldots, B_{k+1}, B_{k+2}, \ldots, B_0\} \) do
8: \( \quad \text{if } MMD^2_t(F, \bigcup_{i=s+1}^{k} B_i \cup \bigcup_{i=0}^{n} B_0) \geq \epsilon_0, \text{ then} \)
9: \( \quad \quad \text{print } \text{"Change before bucket } s \text{ detected at time } t\"
10: \( \quad \text{buckets} \leftarrow B_{s+1}, \ldots, B_0 \quad \triangleright \text{Drop buckets coming before } s \)
11: \( \text{while two buckets have the same size do} \quad \triangleright \text{Update data structure} \)
12: \( \quad \text{Merge buckets following Equation (4) into } B' \)
13: \( \quad \text{Subsample a logarithmic number of observations in } B' \text{ uniformly} \)

The following proposition and its corollary give the value for threshold \( \epsilon_0 \).

**Proposition 2.** Let \( p, q, X, Y \) be defined as before, and assume \( 0 \leq k(x, y) \leq K \), and \( p = q \). Then

\[
P\{MMD_0(F, X, Y) - (K/m + K/n)^{1/2} \geq \epsilon_0\} \leq \exp \left( -\frac{t^2 mn}{2K(m+n)} \right) .
\]

**Proof.** The proof follows [18, Proof A.3] without assuming \( m = n \), see our Appendix A.2. \( \square \)

**Corollary 1.** A hypothesis test of level \( \alpha \) for \( p = q \) has acceptance region

\[
MMD_t(F, X, Y) < \sqrt{\frac{K}{m} + \frac{K}{n}} \left( 1 + \sqrt{2\ln \alpha^{-1}} \right) .
\]

**Proof.** Set \( \alpha = \exp \left( -\frac{t^2 mn}{2K(m+n)} \right) \) and solve for \( t \) to obtain a test of level \( \alpha \). \( \square \)
3.3 Analysis of MMDAW

Algorithm \[\text{Algorithm}_1\] subsamples \(l\) observations in each respective bucket uniformly, where \(2^l\) would be the size of the bucket without sampling. This leads to the question of how the sampling influences the number of terms accumulated in the sums stored with each bucket. The following proposition answers this and reveals the rationale behind combining buckets of exponentially increasing size with the subsampling scheme, i.e., why this approach is better than directly subsampling a share of the data logarithmic in size without using the summary structure.

Illustrative Example. We assume a stream of observations \(x_1, x_2, \ldots\) having a common distribution. Then, MMDAW receives the first observation, \(x_1\), and creates a bucket \(B_0\), storing \(x_1\), \(XX_0 = k(x_1, x_1)\), and \(XY_0 = \emptyset\). For the next observation, \(x_2\), it creates a new bucket \(B_{0'}\), storing \(x_2\), \(XX_{0'} = k(x_2, x_2)\), and \(XY_{0'} = \{k(x_1, x_2)\}\) and detects no change. As \(B_0\) and \(B_{0'}\) have the same size, MMDAW merges them into bucket \(B_1\), storing a sample of size \(\log_2 2 = 1\), e.g., \(x_1\), and computes \(XX_1 = k(x_1, x_1) + k(x_2, x_2) + 2 \cdot k(x_1, x_2)\), following Equation \[\text{Equation}_4\]. As no previous bucket exists, the computation of \(XY_1\) is not required. We see that the number of terms in \(XX_1\) equals four, while \(B_1\) stores only one observation.

Proposition 3. For a bucket of size \(2^l\), the number of terms of the sum \(XX_1\) is

\[
n_{XX_1} = [z^l] -\frac{8z^3 + 2z - 1}{(2z - 1)^3} = 2^{l-1}(l^2 - l + 4), \quad k \geq 1,
\]

i.e., it is given by the coefficient of \(z^l\) in the series expansion of the generating function. Thus, for \(n = 2^l\), we find that the number of terms is

\[
n = \frac{2^l(l-1)}{2} \log_2 n - 2n + 4). \tag{7}
\]

The number of interaction terms \(XY_1\) between buckets of size \(2^l\), i.e., both buckets have the same size, is given by

\[
n_{XY_1} = 2^l(l-1) = n(\log n - 1), \quad l > 1, b_0^1 = 1. \tag{8}
\]

The asymptotic growth of the number of terms \(n_{XX_1}\) is \(O(n \log^2 n)\). If we omit the summary data structure and, to obtain the same memory complexity, directly subsample a logarithmic number of samples instead, the growth would be \(O(\log n)\). Hence, the combination of the summary data structure with the subsampling allows a better approximation of MMD than subsampling alone.

Proof. To simplify notation, we use \(a_l\) for the number of terms in \(XX_1\) in bucket \(l\), and \(b_l^j\) for the number of terms in \(XY_j\) of the sum between buckets \(i\) and \(j\). We start by noticing that \(a_l\) only changes when we merge two buckets, which only happens for buckets of the same size. Both have counts \(a_{l-1}\). We add to this \(2 \cdot b_{l-1}^{j-1}\), see Equation \[\text{Equation}_4\], to obtain the recurrence relation

\[
a_l = \begin{cases} 
1 & \text{if } l = 0, \\
4 & \text{if } l = 1, \\
2 \cdot a_{l-1} + 2 \cdot b_{l-1}^{j-1} & \text{if } l > 1.
\end{cases} \tag{9}
\]

The \(b_l^k\) counting the number of \(XY\) between two buckets of the same size are \(1, 2, 8, 24, \ldots\), i.e., \(b_l = 2^l(l-1), l > 1\) and \(b_0^0 = 1\). We write

\[
a_l = 2 \cdot a_{l-1} + k \cdot 2^l - 2^l + 2 \cdot [l = 0] + 2 \cdot [l = 1], \tag{10}
\]

where the brackets are equal to one if their argument is true and zero otherwise (using Iverson’s convention \[\text{Iverson’s convention}_17\]). Defining ordinary generating function \(A(z) = \sum_l a_l z^l\), multiplying by \(z^l\) and summing on \(l\), we obtain the stated result

\[
A(z) = -\frac{8z^3 + 2z - 1}{(2z - 1)^3} \tag{11}
\]

after some algebra. To extract coefficients, we decompose \(A(z)\) into the terms of the sum \((2z + 2)/(1 - 2z), 2z/(2z - 1)^3, \) and \(-1/(2z - 1)^2\) and apply the General Expansion Theorem for Rational Generating Functions \[\text{Iverson’s convention}_17\].

It follows that Algorithm \[\text{Algorithm}_1\] has a runtime complexity of \(O(\log^2 t)\) per insert operation and a total storage complexity of \(O(\log t)\). Hence, it fulfills the requirements for streaming algorithms.
3.4 Comparison to ADWIN

In contrast to ADWIN [3], MMDAW detects, given a universal kernel, arbitrary changes in distributions, while ADWIN is limited to detecting changes in mean in univariate data. In that sense, our algorithm is more general than ADWIN. Indeed, the following proposition establishes that MMDAW comprises the comparison of means as a special case.

**Proposition 4.** For \( k(x, y) = \langle x, y \rangle \) and \( \mathcal{X} = \mathbb{R} \), Algorithm [7] reduces to the comparison of means.

**Proof.** By the linearity of the (real) scalar product and the binomial theorem

\[
\begin{align*}
\text{MMD}^2_b[\mathcal{F}, X, Y] &= \frac{1}{m^2} \sum_{i,j=1}^{m} \langle x_i, x_j \rangle + \frac{1}{n^2} \sum_{i,j=1}^{n} \langle y_i, y_j \rangle - \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \langle x_i, y_j \rangle \\
&= (\bar{x} - \bar{y})^2.
\end{align*}
\]


4 Experiment Setup

4.1 Data Sets and Data Preparation

In the following, we describe the real-world data sets used here. As only few high-dimensional and annotated change detection data sets are publicly available, we employ well-known classification data sets and interpret them as streaming data (12; 11): We order the observations in each data set by their classes; a change occurs if the class changes. To introduce some variation into the order of change points, we randomly permute the order of the classes before each run (using the same permutation for all algorithms). For preprocessing, we apply min-max scaling to all data sets.

- **CIFAR10** (22), **FashionMNIST** (34), **MNIST** (8). These well-known image data sets have a dimensionality of 1024 (converted to grayscale), 748, and 748. Their numbers of observations are 60000, 70000, and 70000, respectively, and their numbers of classes all equal ten, i.e., each data set has nine change points.

- **Gas** (30). The Gas Sensor Array Drift data set contains 128 features extracted from 16 sensors which were exposed to six gases at various concentration levels. Changes happen when the sensors are exposed to a different gas. It contains 13910 observations and has five change points after reordering.

- **HAR** (2). The Human Activity Recognition with Smartphones data set has 561 features of smartphone accelerometer and gyroscope readings of a person performing six different actions. Changes in the action correspond to change points. This data set has 10299 observations with five change points.

4.2 Evaluation

We use the precision, the recall, the \( F_1 \)-score, and the Mean Time To Detection (MTD), which are common to evaluate change detection algorithms (29; 11). Specifically, we define a true positive (tp) if a change point is detected within \( \Delta_T \) steps of an actual change point. We count a false positive (fp) if a change point is reported, and there is no actual change point within the \( \Delta_T \) previous time steps. If an algorithm does not report a change point within \( \Delta_T \) steps of an actual change point, we count a false negative (fn). We count at most one true positive for each actual change point. With these definitions, the precision is \( \text{Prec} = \frac{\text{tp}}{\text{tp + fp}} \), the recall is \( \text{Rec} = \frac{\text{tp}}{\text{tp + fn}} \), and the \( F_1 \)-score is their harmonic mean \( F_1 = 2 \cdot (\text{Prec} \cdot \text{Rec}) / (\text{Prec} + \text{Rec}) \). MTD is defined as the mean delay between an actual change point and the next reported one (4). To interpret our results, we also report the Percentage of Changes Detected (PCD), i.e., the ratio of the number of reported changes and the number of actual change points. Note that, while some algorithms allow to infer where in the data a change happens, we only evaluate the time at which they report a change.

We run each algorithm with ten different permutations of each data set, on a server running Ubuntu 20.04 with 124GB RAM, and 32 cores with 2GHz each. We report the average score per data set together with its standard deviation.
4.3 Configuration and Competitors

To obtain a fair comparison, we run a grid parameter search per data set and algorithm and report the best result w.r.t. the $F_1$-score. We note that such an optimization is rarely feasible in practice, as ground-truth data might not be available, and algorithms featuring fewer parameters often are preferable. To ensure reproducibility, Table 1 lists all parameters tested. For MMDAW, we use the Gaussian kernel, i.e., $k(x, y) = \exp(-\gamma \|x - y\|^2)$ and set $\gamma$ using the median heuristic on the first 100 observations. The Gaussian kernel is universal and allows, given enough data, to detect any change in distribution. We also give the first 100 observations to competitors requiring data to estimate further parameters (IBDD, WATCH) upfront. We make our implementations of the competitors, together with the implementation of MMDAW, available on our GitHub account.

Table 1: Configuration of our parameter grid for the parameter optimization.

| Algorithm | Parameters | Parameter values |
|-----------|------------|------------------|
| MMDAW     | $\alpha, b$ | $\alpha \in \{0.001, 0.01, 0.1, 0.2\}, b = 2$ |
| ADWINK    | $\delta, k$ | $\delta = 0.05, k \in \{0.01, 0.02, 0.05, 0.1, 0.2\}$ |
| D3        | $\omega, \rho, \tau, \text{depth}$ | $\omega \in \{100, 200, 500\}, \rho \in \{0.1, 0.3, 0.5\}, \tau \in \{0.7, 0.8, 0.9\}, \text{depth} = 1$ |
| IBDD      | $m, \omega$ | $m \in \{10, 20, 50, 100\}, \omega \in \{100, 200, 300\}$ |
| WATCH     | $\epsilon, \kappa, \mu, \omega$ | $\epsilon \in \{2, 3\}, \kappa = 100, \mu \in \{1000, 2000\}, \omega \in \{500, 1000\}$ |

5 Results

Figure 1 shows our results w.r.t. $F_1$-score, precision and recall. As $\Delta_T$ is an evaluation-specific parameter, we vary it relative to the average distance between change points by a factor $\beta$: Given a data set of length $N$ with $n$ changes, we set $\Delta_T = \beta \cdot N / (n + 1)$. For $\beta = 1$, i.e., $\Delta_T$ is equal to the average number of steps between change points in each respective data set, MMDAW achieves a higher $F_1$-score than all competitors on all data sets, showing the best balance between precision and recall. Other approaches either have an unreasonably low precision (i.e., less than 20%), or an inferior recall and precision, down to a few exceptions. For $\beta = 1/2$, MMDAW achieves the best result on 4 out of 5 data sets; for $\beta = 1/4$, it achieves the best result on 3 out of 5 data sets. For precision, we obtain similar results: Here, MMDAW shows the best performance on 4 out of 5, 3 out of 5, and 3 out of 5 data sets, respectively. Regarding recall, IBDD and WATCH show the best performance. However, as both have low precision, this indicates that they report too many false positives.
We verify this behavior in Figure 2. For PCD, results closer to 100% are better. Here, MMDAW is on par with the closest competitors and consistently, i.e., with low variance, detects an approximately correct number of change points; IBDD and WATCH indeed detect too many change points. For MTD, lower values are better. Here, MMDAW on average also achieves competitive results.

Figure 2: Mean of PCD (log scale) and of MTD. Vertical bars show the standard deviation.

Interpreting the above, the reduction of $\Delta_T$ leading to a decrease of the $F_1$-score indicates that MMDAW as is has some delay when detecting changes. The MTD plot seems to confirm this. To reduce the delay, one may defer the subsampling, to keep more samples per bucket. Nevertheless, MMDAW achieves competitive results w.r.t. the $F_1$-score in all cases and, as Figure 2 tells us, it is also competitive w.r.t. the PCD and MTD.

6 Conclusions

In this paper, we tackle the long-standing problem of change detection in data streams by using the principled approach of two-sample hypothesis testing. We observe that, while MMD features an appropriate hypothesis test, its standard estimator does not fulfill the streaming requirements. To address this issue, we introduce a new data structure together with a change detection algorithm, dubbed MMDAW, which allow estimating MMD with low runtime and memory complexity in an online fashion. Our experiments on standard benchmark data show that MMDAW has the best $F_1$-score on most data sets and in particular high precision. The usefulness of our algorithm is not only due to its good performance. MMDAW has two parameters, and only one of them requires tuning. This parameter, $\alpha$, corresponds to the power of the statistical test, which makes it intuitive to set and simplifies MMDAW’s application to real-world use cases.

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A Appendix: Formal Proofs

A.1 Preliminary Theorems

We need the following fact, also known as McDiarmid’s inequality, for example found in (31):

**Theorem 1** (Bounded differences inequality). Let $X_1, \ldots, X_n$ be independent random variables. Let $f : \mathbb{R}^n \to \mathbb{R}$ be a measurable function. Assume that the value of $f(x)$ can change by at most $c_i > 0$ under an arbitrary change of a single coordinate of $x \in \mathbb{R}^n$. Then, for any $t > 0$, we have

$$
\mathbb{P}\{f(X) - \mathbb{E}f(X) \geq t\} \leq \exp\left(-\frac{2t^2}{\sum_{i=1}^{n} c_i^2}\right)
$$

where $X = (X_1, \ldots, X_n)$.

A.2 Bounds of Hypothesis Test

Here, we prove the result of Proposition 2 by following the proof of Theorem 8 in (18) but without assuming that $m = n$, i.e., both samples may be of different sizes. Note that we recover the original result in the case that $m = n$. To ensure self-containedness, we restate the necessary results of (18).

First, we bound the difference of MMD$_b(F, X, Y)$ to its expected value. Changing a single one of either $x_i$ or $y_j$ in this function results in changes of at most $2\sqrt{K}/m$, and $2\sqrt{K}/n$, giving

$$
\sum_{i=1}^{n+m} c_i^2 = 4K \frac{n + m}{mn}.
$$

We now apply the Bounded Differences Inequality to obtain

$$
\mathbb{P}\{\text{MMD}_b(F, X, Y) - \mathbb{E}\text{MMD}_b(F, X, Y) \geq t\} \leq \exp\left(-\frac{t^2 mn}{2K(m + n)}\right).
$$

The last step is to bound the expectation, and we have

$$
\mathbb{E}_{X, Y} \left[ \sup_{f \in F} \left( \frac{1}{m} \sum_{i=1}^{m} f(x_i) - \frac{1}{n} \sum_{j=1}^{n} f(y_j) \right) \right]
$$

$$
= \mathbb{E}_{X, Y} \left[ \left\| \frac{1}{m} \sum_{i=1}^{m} \Phi(x_i) - \frac{1}{n} \sum_{j=1}^{n} \Phi(y_j) \right\| \right]
$$

$$
= \mathbb{E}_{X, Y} \left[ \left( \frac{1}{m^2} \sum_{i=1}^{m} \sum_{j=1}^{m} k(x_i, x_j) + \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} k(y_i, y_j) - \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} k(x_i, y_j) - \frac{1}{mn} \sum_{j=1}^{n} \sum_{i=1}^{m} k(y_j, x_i) \right)^{\frac{1}{2}} \right]
$$

$$
\leq \left( \frac{1}{m} \mathbb{E}_x k(x, x) + \frac{1}{n} \mathbb{E}_y k(y, y) + \frac{1}{m} (m - 1) \mathbb{E}_{x,y} k(x, y) + \frac{1}{n} (n - 1) \mathbb{E}_{x,y} k(y, x) - 2 \mathbb{E}_{x,y} k(x, y) \right)^{\frac{1}{2}}
$$

$$
= \left( \frac{1}{m} \mathbb{E}_x k(x, x) + \frac{1}{n} \mathbb{E}_y k(y, y) - \frac{1}{m} \mathbb{E}_{x,y} k(x, y) - \frac{1}{n} \mathbb{E}_{x,y} k(x, y) \right)^{\frac{1}{2}}
$$

$$
= \left( \frac{1}{m} \mathbb{E}_{x,y} [k(x, x) - k(x, y)] + \frac{1}{n} \mathbb{E}_{x,y} [k(x, x) - k(x, y)] \right)^{\frac{1}{2}}
$$

$$
\leq \left( \frac{K}{m} + \frac{K}{n} \right)^{\frac{1}{2}}.
$$

Inserting this into the previous inequality, we obtain the stated result.