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# Enabling the Visualization of Distributional Shifts using Shapley Values\*

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## Abstract

In streaming data, distributional shifts can appear both in the univariate dimensions and in the joint distributions with the labels. However, in many real-time scenarios, labels are often either missing or delayed; Unsupervised drift detection methods are desired in those applications.

We design slidSHAPs, a novel representation method for unlabelled data streams. Commonly known in machine learning models, Shapley values offer a way to exploit correlation dependencies among random variables; We develop an unsupervised sliding Shapley value series for categorical time series representing the data stream in a newly defined latent space and track the feature correlation changes.

The slidSHAP series allows us to track how distributional shifts affect the correlations among the input variables independently from any kind of labeling. We show how abrupt distributional shifts in the input variables are transformed into smoother changes in the slidSHAP series, allowing for an intuitive visualization of the shifts when they are not observable in the original data.

## 1 Introduction

Time series analysis includes forecasting, anomaly detection, and concept drift identification. Concept drifts in time series refer both to distributional changes in the labels and in the input variables of the time series; Distributional shifts in the input variables gain traction in the *unsupervised* case when labels are not available, delayed and when unreliable or expensive to obtain.

Commonly used in machine learning applications, Shapley values gained increased popularity [25]. Not yet widely spread in time series, they are recently timidly appearing for anomaly detection, label prediction, and interpretability [5, 31, 26, 30]. The challenge to face in streaming data is the pairing of Shapley values as importance scores with the time-dependence. Distributional shifts have not yet been fairly explored using Shapley values; While some attempts refer to drifts in label-input variables distribution, to the best of our knowledge, none contextualize them for shifts in the input variables. Due to the chaotic structure of the data streams, changes in correlation among input variables can be hard to visualize, making the detection itself a jump of trust in the concept drift detector. Hence, we introduce the slidSHAP series, a time-dependent series representing the distributions and correlations among subsets of the streaming data's input variables. Based on Shapley Values, we obtain an unsupervised tool for visualizing and detecting distributional shifts in the original  $N$ -dimensional time series through a new  $N$ -dimensional latent space. This preliminary work is a representation method for unlabeled discrete time series; Although we now focus on time series whose dimension assumes a finite number of values, future work generalizes the approach to a broader application.

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## 2 Methods

A cooperative game is a pair  $(P, \nu)$  where  $P = \{X_1, \dots, X_N\}$  is the set of players and  $\nu$  a value function, i.e., a set function  $\nu : \mathcal{P}(P) \rightarrow \mathbb{R}_+$ . Shapley values SV [27] are computed for each player  $X_i \in P$  as

$$\phi(X_i) = \sum_{A \subseteq P \setminus \{X_i\}} k_A \cdot (\nu(A \cup \{X_i\}) - \nu(A)) \quad (1)$$

where  $k_A$  depends on  $N$  and the size of  $A$ . SVs have been used as a mean for achieving interpretability of black-box models [17, 28] but, more generally, they represent a way of distributing resources among players in a game. Balestra et al. [4] proposed SVs within an unsupervised feature selection method; the authors used them to encode the structure and the correlations within subsets of features of an unlabelled tabular data set with categorical entries. Given a set of  $N$  discrete random variables  $F = \{X_1, \dots, X_N\}$ , the authors propose to interpret  $F$  as a set of players; In order to encode the data structure and the correlations within subsets of  $F$ , they argued in favor of using as value function a correlation metric. They proposed for their categorical context the total correlation, i.e.,

$$\nu(A) = H(A) - \sum_{X \in A} H(X) \quad (2)$$

where  $H(\cdot)$  is the discrete Shannon entropy [4]. The encoding of the correlations using the total correlation and the use of Shapley values enables to extract information from the data set based on the correlations' structure; the result is that features obtaining high Shapley values are highly correlated with subsets of the other variables while features with lower Shapley values are uncorrelated with the other variables.

### 2.1 Time series and sliding windows

Let  $X = (X_1, \dots, X_N)$  be a multivariate  $N$ -dimensional discrete time series,  $X_i$  the  $i$ -th univariate dimension of the time series. We indicate with  $t_1$  the first timestamp on which the time series is defined. For each timestamp  $t_k > t_1$ ,  $X(t_k)$  is a  $N$ -dimensional vector of discrete values, i.e.,  $X_i(t_k) \in D_i$  and the cardinality of  $D_i$  is finite.

We define *overlapping sliding windows* as a series of time windows  $\{w_s\}_{s \in \mathbb{N}}$  through a window length  $d$  and overlap  $a$  among adjacent windows, i.e.,

$$w_s = \{t_{s(d-a)}, \dots, t_{s(d-a)+d-1}\}. \quad (3)$$

Each window  $w_s$  contains  $d$  timestamps, and  $a$  is the number of timestamps lying in the overlap among adjacent windows, i.e.,  $|w_s \cap w_{s+1}| = a$  for each  $s \in \mathbb{N}$ . After fixing  $a$  and  $d$ , at the current timestamp  $t_T$  we have created  $M(T) = \lfloor \frac{T-d+1}{d-a} \rfloor$  time windows; hence, for a fixed windows' length  $d$ , the larger is the overlap  $a$ , the higher the number of windows created and for fixed overlap  $a$ , the number of windows decreases for increasing  $d$ . Note that  $a, d \in \mathbb{N}_+$ .

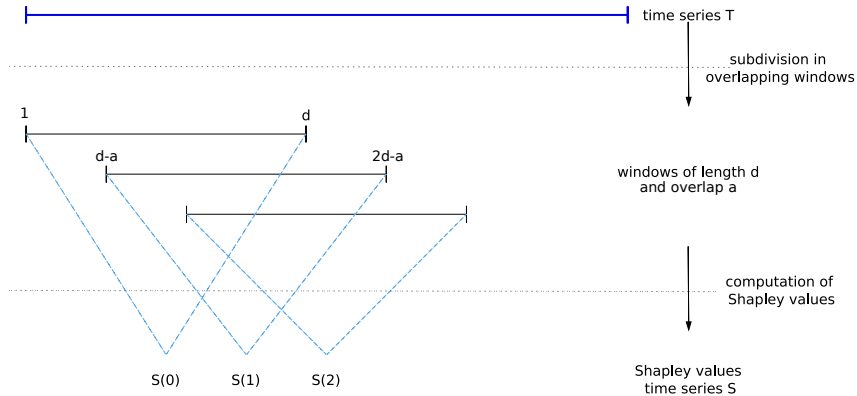


Figure 1: Construction of the slidSHAPs.

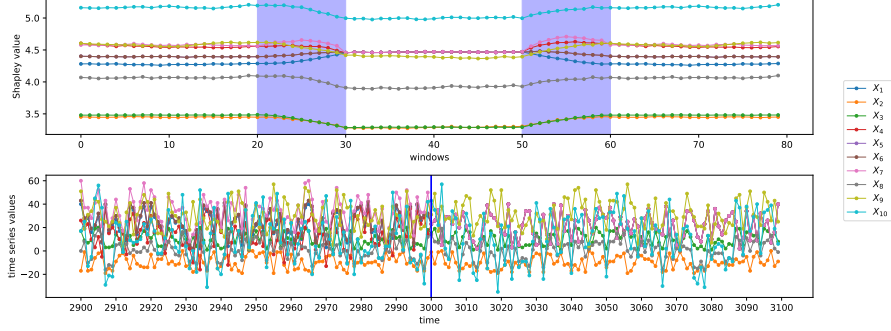


Figure 2: COR3: In the upper plot, the slidSHAP series; in the lower plot, the original time series in the interval  $\{2900, \dots, 3100\}$  where the distributional shifts happen.

## 2.2 slidSHAPs

Given a multivariate time series  $X$  with  $N$ -dimensions we can interpret the value the  $i$ -th dimension at timestamp  $t_k$   $X_i(t_k)$  as the realization of a discrete (categorical) random variable  $X_i$ ; hence, given the set of timestamps  $\{t_1, \dots, t_T\}$ ,  $\{X_i(t_1), \dots, X_i(t_T)\}$  are  $T$  independent realizations of the random variable  $X_i$ . Similarly, we can interpret  $\{X(t_1), \dots, X(t_T)\}$  as the set of realizations of a  $N$ -dimensional discrete random variable. This interpretation allows us to study the correlations among the univariate dimensions of  $X$ .

We interpret the realizations of a time series on a time window  $w_s$  as a discrete tabular data set with  $N$  columns and  $d$  rows; this allows us to compute a Shapley value for each column, i.e., for each univariate dimension of the time series using [4]. Our goal remains the one of visualizing the correlations' structure among dimensions of streaming data; thus, we want to keep a trace of the distributional changes over time. We use the sliding time windows  $\{w_s\}_{s \in \mathbb{N}}$  defined in Section 2.1 and compute Shapley values of the univariate dimensions of  $X$  when restricted to the  $w_s$ s; Hence, we compute the Shapley values for each univariate dimension  $X_i$  of the streaming data in the time window  $w_s$ , i.e.,  $S_i(s) = \phi(X_{w_s}^i)$ . For each time window  $w_s$ , we obtain a vector of Shapley values  $S(s) = [S_1(s), \dots, S_N(s)] \in \mathbb{R}^N$  and each  $S_i(s)$  consider the correlations of  $X_i$  with the other dimensions of the time series in  $w_s$ .

As described in Section 2.1, the computation of the Shapley values inherits from the  $w_s$  the same time-dependency. Figure 1 represents a visual schema for the slidSHAPs series construction process. From the original discrete time series  $X$  assuming finite values, we extrapolate information about the univariate dimensions' correlations and transfer the structure of the data stream to a new  $N$ -dimensional real-valued series, i.e., each slidSHAP value is a  $N$ -dimensional real-valued vector. We interpret the space on which the slidSHAP values are defined as a latent space where we have projected the correlation structure of the original time series. As the sliding windows are partly overlapping, given two close-by indices  $s_1, s_2$ , the information conveyed by  $S(s_1)$  and  $S(s_2)$  relate to partly overlapping time windows of the original time series  $X$ ; Hence, the set up of the parameters  $a$  and  $d$  for the windows' creation is essential to set up the *granularity* for the Shapley values' computations.

Finally, we underline that the slidSHAP series is not dependent on the same time notion of the original time series; when we write  $S(s)$ ,  $s$  represents the index of the time window on which the Shapley values have been computed, i.e.,  $S(s)$  is the vector of Shapley values in the time window  $w_s = \{t_{s(d-a)}, \dots, t_{s(d-a)+d-1}\}$  while  $X(t_k)$  is the value of the time series at the time stamp  $t_k$  and it is a  $N$ -dimensional discrete-valued vector.

## 2.3 Distributional shifts in the univariate dimensions

When dealing with real-world time series, often only a few of the input variables are subject to distributional changes; on the other hand, those changes could affect the correlation structure of the whole set of input variables. We use slidSHAPs as an unsupervised tool for unlabelled time series obtained *sliding* over time windows of fixed amplitude to visualize the correlation structure in the time series. Targeting to detect distributional shifts of the input variables in an unsupervised manner,

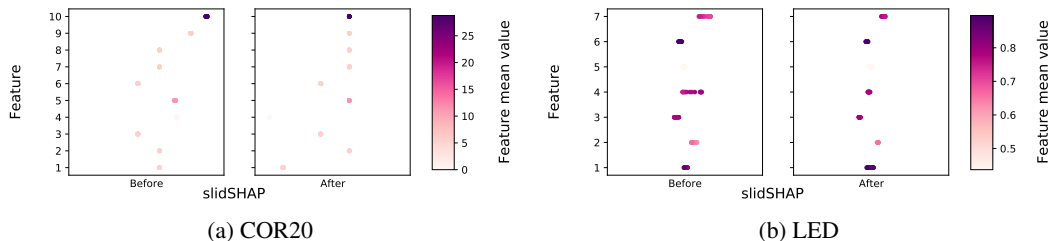


Figure 3: Feature importance before and after the first concept drift in each dataset; The color represents the average value of each sliding window corresponding to the slidSHAP value.

we employ the non-parametric and distribution-free two-sample Kolmogorov-Smirnov Test (K-S Test) and the classical t-test. We slide windows on the slidSHAP series and perform the statistical testing on each of the univariate variables following the approach proposed in [23].

### 3 Experiments

**Datasets:** We use synthetic datasets and a common benchmarking dataset to show the performances of slidSHAPs. We first create two 10-dimensional synthetic datasets; in COR3, the correlations among the input variable change every 3000 data instances, while in COR20 the changes happen every 5000 instances. Furthermore, we employ the standard benchmark dataset LED where distributional shifts happen every 9000 instances. The concepts underlying the input variables’ distributions in all datasets change abruptly at specific time stamps. More details on the dataset construction and their characteristics can be found in Appendix C.

**Results:** We used the datasets to show our representation of the time series correlations on the latent space. Figure 2 shows how the slidSHAP series are visually more appealing than the original data streams in visualizing distributional shifts. In COR3 the distributional shifts happen at the time stamps 3000 and 6000. Using slidSHAPs ( $a = 900, d = 1000$ ), we see that the abrupt changes are smoothed out in the upper plot; in the lower plot, the original time series data, where, although containing a significant distributional shift, it is not possible to observe any. Figure 5 (in the Appendix) shows the slidSHAP series for the other two datasets; we plotted dashed lines, where the shifts happen, and where they have been detected using statistical testing.

We checked for changes in the slidSHAP series and plotted them against the changes in the range of values in which the dimensions of the time series vary. The values of the slidSHAPs in the time windows are averaged and color-coded in the plots. Intuitively, a distributional drift in the input space causes a change in the slidSHAP values, which can be detected as concept drift (e.g.,  $X_4$  and  $X_7$  in LED). Figure 3 shows this comparison in the LED and COR20 datasets before and after the first distributional shift. Furthermore, the slidSHAP series also clearly show the shifts of some non-observable input space drifts, where the amplitude of features stays in the same range while the feature correlation changes. Significant changes can still be observed in the slidSHAP values (e.g.,  $X_{10}$  in COR20).

### 4 Discussion and conclusions

In real-time applications, streaming data appear with or without labels. In this second case, distributional shifts can appear in one or more of the input dimensions. We propose the slidSHAP series, a new representation of the time-dependent correlations among input variables of unlabelled time series; slidSHAPs allow for visualizing distributional changes in the input features as well as keeping track of the correlations changes among the input dimensions. We base our approach on a feature correlation-based value function, hence being completely unsupervised. The visualization of the slidSHAP series provides additional understanding of the often non-observable correlational shifts in the input variables. The experimental results show our approach’s effectiveness in various synthetic data sets. Future work will include the study slidSHAPs in real-world scenarios.

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## A Related work

Several approaches are proposed in the state-of-the-art literature to deal with concept drifts in time series. Many approaches are based on prediction error rate, where the distributional shift appears in  $\mathbb{P}(y|X)$  instead of in the input variables  $\mathbb{P}(X)$  [16, 7, 15]. However, the increasing number of scenarios where time series data are collected and no labels are provided increased fast; the necessity of dealing with distributional shifts on input variables forced the development of unsupervised concept drift detection methods. Among the several representation learning approaches used for detecting drift, we recall the most common. Bifet et al. [7] use the mean values of defined adaptive windows to represent the univariate dimensions of the time series, while Cavalcante et al. [8] employ a few linear and non-linear features to represent the whole time series. Da Costa et al. [10] propose to apply multidimensional Fourier transformation to get information about the frequency domain. More recently, a combination of multiple statistical features of the time series data has been proposed as meta-information vectors [16]. Other approaches measure the distributional discrepancy between data from different periods: It is the case in HDDDM [12] that measures the Hellinger distance between two distributions and Dasu et al. [11] that partition data via constructing a Kdq-Tree and generalize the Kulldorff’s spatial scan statistic, allowing to identify regions in the Kdq-Tree with the most considerable changes quantitatively. Unfortunately, all the methods above do not explicitly monitor the correlation changes between features and may miss some drifts appearing in this domain. In the state-of-the-art literature, feature correlation in time series is mainly studied using covariance. Attempts to extend the limitation of using only covariance appeared in [2], where both mean, and covariance is used to represent the concepts in multivariate data streams. Qahtan et al. [22] detect concept drifts using the covariance matrix, tracking covariance changes in a transformed artificial low-dimensional space obtained applying PCA on the original time series data; thus, their approach does not explicitly reflect the correlation change in the original input space. A few works are worth to be mentioned where Shapley values have been applied for drift detection: Zheng et al. [33] show that the traditional Shapley value in a classification context can also be used for drift detection. Zhao et al. [32] employ Wasserstein distance and Energy distance to detect feature drifts without label and apply Shapley value and LIME [24] as post-hoc interpretation for the detected drifts. Moreover, supervised and unsupervised distributional shift detection are of great importance in many critical contexts, for example, in time series for health applications. Applications vary among surgery prediction, medical triage, heart diseases prediction [1, 6, 13]. Also, in the medical context, unsupervised distributional shifts are getting more and more importance [14].

Introduced by Shapley in 1953 [27], Coalitional Game Theory became popular in machine learning in the early 2000s. Cohen et al. [9] introduced Shapley values as a fair evaluation for features’ contributions in order to achieve supervised feature selection. Later, Shapley values were applied to interpret black-box models by Lundberg et al. [17]. The success of their use in machine learning, brought to further extensions and applications both in the machine learning community [20, 21] and in bioinformatics [29, 18]. In recent years, Shapley values also started being applied to time series data. TimeSHAP [5] being one of the first extensions of Shapley values to time series is based on KernelSHAP [17]; The authors propose a method to compute Shapley values to get event- and feature-level explanations and provide insights on reducing Shapley computation’s computational complexity. Saluja et al. [26] propose an application for prediction and forecasting of the income of a consulting company; Antwarg et al. [3] introduce two different methods. The first approach looks for anomalies through the reconstruction error and the autoencoder; the method is based on comparing the Shapley values of the original features and the reconstructed ones. Taikesh [30] studies the difference among Shapley values of single instances before and after a change in one feature that makes the instance itself anomalous. Nguyen et al. [19] explain the anomalies by analyzing the gradients to identify the main features affecting the anomalies.

## B Experiments

**Evaluation metric** For each synthetic dataset, the slidSHAP series are computed with various combinations of sliding window lengths and overlaps, i.e., the parameters  $a$  and  $d$ . In order to evaluate the concept drift detection on the newly defined slidSHAP series, we need to include labels from the ground truth from the original time series; since we built the time series with drifts happening at specific timestamps, we need to transfer the induced labeling to the new slidSHAP series.

### B.1 Distributional shifts detection

We apply a sliding window with window length  $d = 1000$  over each time series dataset, and we examine the detection performance under different sliding window overlap sizes  $a \in \{990, 900, 500\}$ . We conduct the K-S tests at significance level  $\alpha = 0.05$  with buffers of length 5. As shown in Table 1, higher  $a$  leads to more false positive detection and slightly better accuracy. We are able to figure out that the model becomes more sensitive to drifts due to the increase of slidSHAP curve smoothness.

Table 1: Drift detection performance ( $\alpha = 0.05$ )

	$a = 990$				$a = 900$				$a = 500$			
	TP	FP	FN	ACC	TP	FP	FN	ACC	TP	FP	FN	ACC
COR3	0	6	2	0.990	1	2	1	0.958	1	1	1	0.714
COR20	7	115	12	0.987	19	43	0	0.956	17	1	2	0.984
LED	0	22	9	0.997	3	5	6	0.988	2	2	7	0.947

The step size is considered a factor of granularity in the slidSHAPs. For each concept drift, a smaller  $d$  leads to more sliding windows, thus more slidSHAP instances containing the same drift event so that the trend in slidSHAPs becomes smoother. As in Figure 4, we plot the nearby slidSHAP values of the first distributional shift in each dataset. As the overlap size  $a$  decreases, the shift becomes more abrupt in the slidSHAP space.

Note that even if only a few dimensions are affected by distributional shifts, all slidSHAPs are affected. This happens as Shapley values evaluate how the dimensions are correlated; when some dimension  $X_i$  shifts to another distribution, all the other input dimensions which were correlated with  $X_i$  or that are correlated with  $X_i$  after the shift has happened are affected (cf. Appendix C).

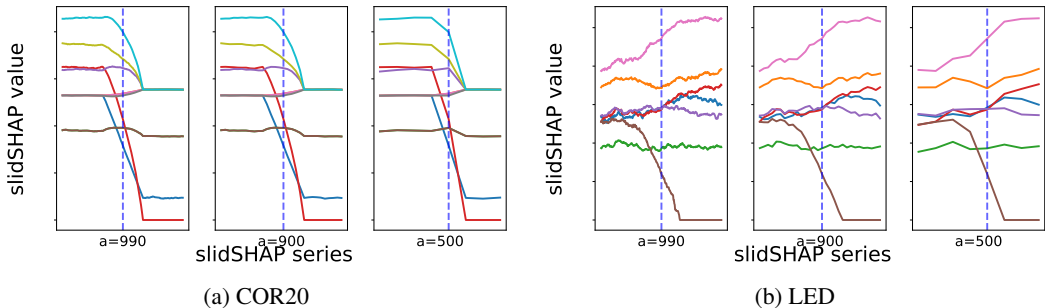


Figure 4: slidSHAP evolution of the first concept drift in each dataset: Each solid line denotes the slidSHAP values on a feature dimension. The dashed blue line depicts the first concept drift position.

### B.2 slidSHAP visualization

In Figure 5, we visualize complete slidSHAPs series.



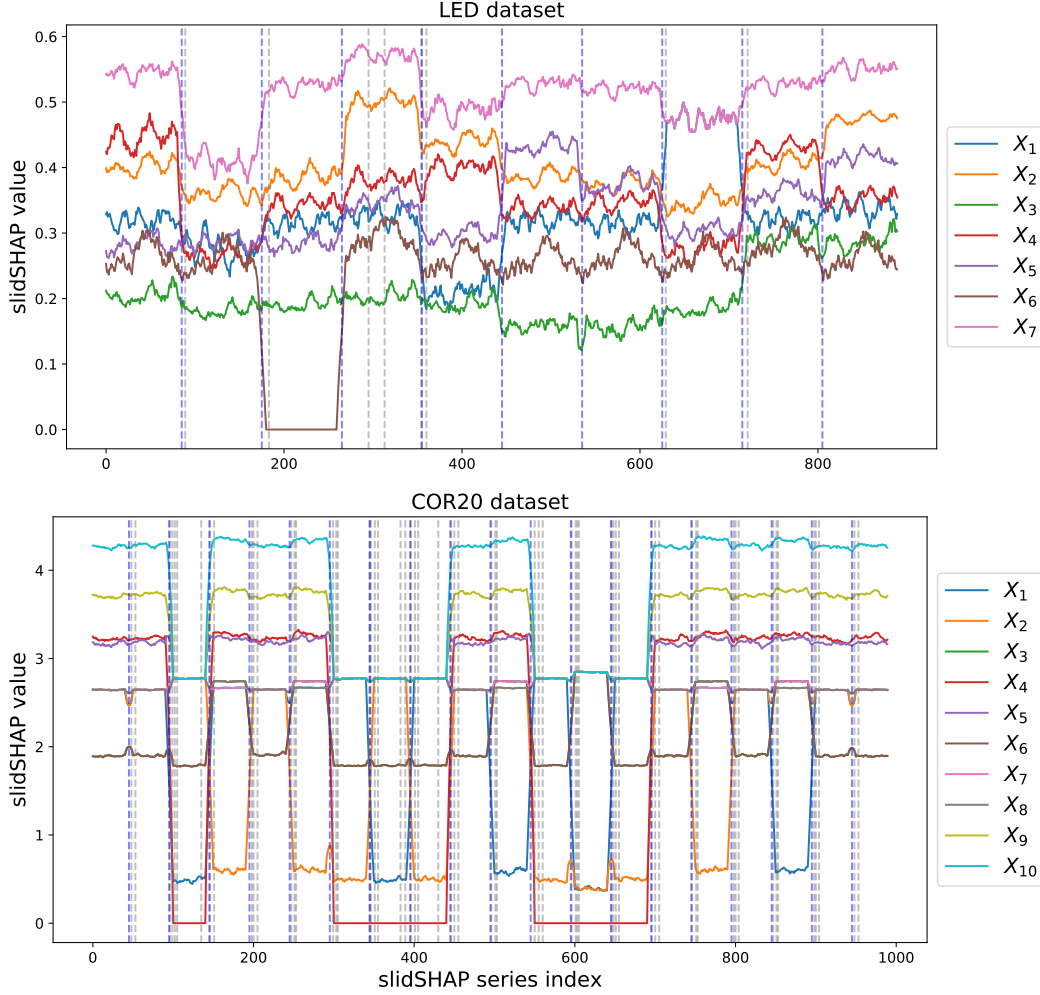


Figure 5: slidSHAPs of the LED dataset and the COR20 dataset both using windows' length 1000 and overlap = 100. The blue dashed lines indicate the true position of the distributional drifts, while the grey dashed lines are where they have been detected using the t-test on the slidSHAPs.

## C Dataset details

COR3 contains 9000 instances and 10 dimensions; two distributional shifts happen respectively at timestamp 3000 and 6000, involving only 3 of the dimensions of the time series data. In COR3, the first 3 dimensions are randomly and individually sampled integers,  $X_1 \in [1, 30]$ ,  $X_2 \in [-20, -10]$ ,  $X_3 \in [1, 10]$ . Moreover, we define an integer random noise  $\epsilon \in [1, 3]$ . The remaining dimensions are correlated with the first dimensions,

- $X_4 = X_1 - X_3 + \epsilon$
- $X_5 = X_1 + \epsilon$
- $X_6 = X_1 + \epsilon$
- $X_7 = X_1 + X_3 + \epsilon$
- $X_8 = X_2 + X_3$
- $X_9 = 2 \times X_3 - X_2$
- $X_{10} = 2 \times X_2 + 3 \times X_3$

3000 data instances are generated in this way in the first 3000 timestamps. To simulate a distributional shift, we change the following four dimensions to,

- $X_4 = X_1$
- $X_5 = X_1$
- $X_6 = X_1$
- $X_7 = X_1$

The new concept also lasts 3000 timestamps. Finally, the first concept reappears again as the third distributional shift. The three concepts are concatenated directly at the timestamps 3000 and 6000, respectively.

COR20 contains 20 different 10-dimensional concept, each concept lasts 10000 timestamps. The first 3 dimensions are also randomly and individually sampled integers,  $d1, X_2, X_3 \in [1, 10]$ . To generate each concept, we randomly select  $X_a, X_b \in \{X_1, X_2, X_3\}$ , and define the remaining dimensions as,

- $X_4 = X_a - X_b$
- $X_5 = X_a + X_b$
- $X_6 = X_3$
- $X_7 = X_a$
- $X_8 = X_b$
- $X_9 = 2 \times X_a - X_b$
- $X_{10} = 3 \times X_a + 2 \times X_b$

All concepts are concatenated directly as abrupt concept drift. To be noticed, if  $X_a = X_b$ ,  $X_4$  becomes constant. We enforce that adjacent concepts cannot have the same  $X_a$  and  $X_b$ . The first concept reappears at every 5th concept.