APPLYING KERNEL CHANGE POINT DETECTION TO FINANCIAL MARKETS

Tyler Manning-Dahan

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By: **Tyler Manning-Dahan**

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Abstract

Applying Kernel Change Point Detection to Financial Markets

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Text of abstract.

Acknowledgments

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Chapter 1

Introduction

1.1 Motivation

In the first half of the twentieth century, Walter Shewart pioneered the use of statistical control charts for detecting real-time changes in variation. Shewart was interested in reducing the unexpected causes of variation in the manufacturing processes that produced faulty manufacturing equipment [54]. Shewart's method involved charting the process measurements over time and detecting when a statistical process was no longer exhibiting an expected level of variation. Once this detection occurred, the process was stopped and was not restarted until the cause of the variation was fixed. Shewart's control charts were one of the first formal methods to solve the problem of detecting changes in a distribution of a sequence of random variables. This problem is now known more generally as the *change point detection problem*. Many industries make use of change point techniques for real-time decision support systems. The following are a few motivating examples.

1.1.1 Health Care

Health care is an important area for quickly detecting signal changes. Some recent studies include applications to heart rate monitoring [63] [57], epilepsy signal segmentation [41], and multi-modal MRI lesion detection [6] to name a few. Quickly detecting changes to a patient's health is absolutely necessary for any system to be of practical use. However, this quick detection must be balanced with high accuracy as

false positives or missed detections could have life-threatening consequences. There-fore, balancing missed change points with falsely identified change points is a central theme to online change point detection.

1.1.2 Financial Applications

The application of accurate and timely change point detection is popular in the fi-nance sector where shifts in asset prices can suddenly happen. Change point detection is particularly hard in financial applications because of the non-stationary data typ-ically observed in asset price time series. A common goal is detecting key, historical moments in the market such as stock market crashes [3] or the sub-prime mortgage crisis [66]. Note, in the financial literature, change points are also referred to as structural breaks, but for this thesis we will use the broader term change points.

An online, quick detection technique is proposed in [48], where a modified Shiryaev - Roberts procedure is used to detect a change point in a single stock's daily returns. See Figure 1 for the kind of of change points the authors try to detect. They compare their non-parametric method with other classic control chart methods using speed of detection and false alarm rate as measures of performance.

Figure 1: Daily stock prices (**top**) and daily returns (**bottom**) for Apple Inc. (NYSE: AAPL) for the period from January 1, 2006 through February 28, 2020.
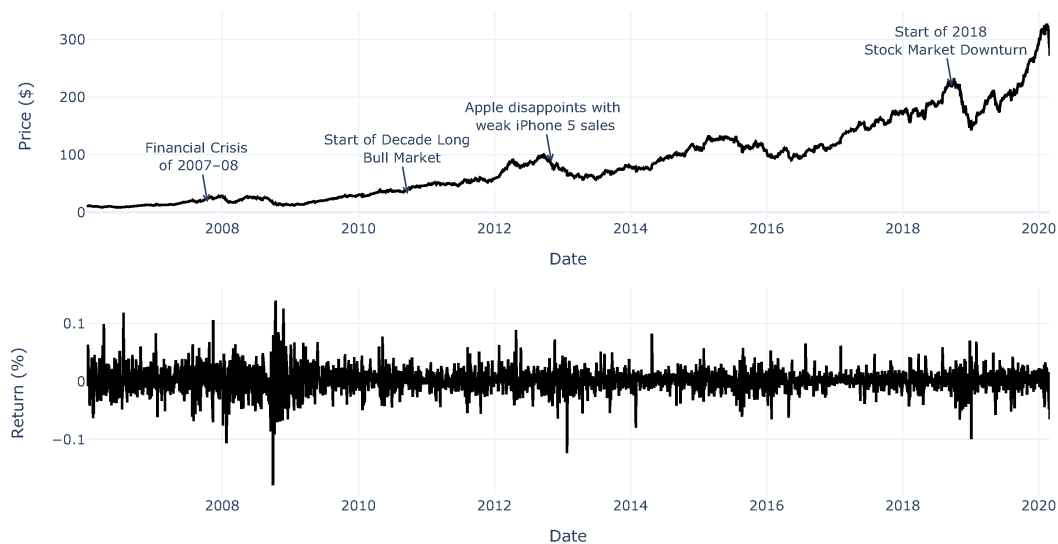
Detecting changes in variance is explored in [33]. The authors propose an offline change point algorithm that minimizes a global cost function by using an adaptive regularization function. The algorithm is applied to the absolute returns of the FTSE 100 stock index and the US dollar-Japanese Yen foreign intra-day exchange rate to detect changes in asset price volatility. The change points identified in the FTSE 100 coincided with key market events such as the stock market crash that occurred on October 14th, 1987 and breaking the 5000 price barrier in August 1997.

For more applications to options markets and arbitrage opportunities, see section 1.3.6 of [59].

1.2 Characteristics of the change point problem

A number of surveys of the literature already exist [1] [46], therefore we will not cover all existing methods but rather touch upon several, important factors to consider when approaching a change point detection problem. Across the literature, these factors determine what methods are available to practitioners.

The first factor is selecting between *parametric* and *non-parametric* techniques. Deciding between these two broad techniques is dependent on the prior knowledge one wants to encode into the problem. For example, if it is known that data is generated by a distribution from an exponential family of distributions, then the problem can be subsetted from the space of all possible distributions to a smaller space of distributions. For example, Shewart control charts and CUSUM change point techniques are both parametric techniques based on the Gaussian-family of distributions [47] [10]. In other settings, it is not possible to leverage information about the data and non-parametric techniques must be used instead [7].

The second factor is deciding whether change points should be detected *offline* or *online*. Some algorithms are offline—also referred to as batch algorithms or retrospective or *posteriori* change point detection—and they are applied in an ex-post fashion after the dataset has been completely acquired [61]. If change points must be detected as soon as possible, then waiting for the entire dataset to be acquired is not feasible and methods that operate on data streams must be used. Methods that fall into the category are referred to as online change point detection methods. The aforementioned Shewart control chart and CUSUM algorithm are both designed

for data that is streamed in real-time. In the statistical literature, online methods of change point detection are also referred to sequential change point detection [59]. For this thesis, the terms will be used interchangeably.

The third factor is determining if there are multiple change points or only one change point to detect. This is an important factor for offline change point detection where the decision to detect one or more change points is often chosen at the outset [28]. Detecting multiple change points could also be relevant for the online case if a situation arises where the window of time series under consideration may contain more than one change point. However, most online change point methods are designed to detect a single change point at a time.

Finally, the last factor to address is determining what statistical changes a change point detection algorithm should detect. Many methods focus solely on detecting changes in the mean of a distribution [35] or changes in variance [22] [27]. Methods like kernel change point detection do not focus on detecting a specific statistical parameter, but rather detecting that a change occurred in some moment of the distribution [2]. This is especially useful in situations where very little is known about the data.

This thesis will concern itself with online change point detection, where data is received in a streaming nature. We assume no prior distributional characteristics on the data and operate in a completely non-parametric setting.

1.3   Our Contributions

The contributions of this work are several fold. First, to our knowledge, no paper has explored the state of the book over time or applied change point detection techniques to order book liquidity levels. Second, given the strong emphasis of theoretical results in the change point detection community, we test several, recent online kernel change point algorithms on synthetic data and real-world data. Classification error as well as time to detection are compared across the various methods. The focus of recent algorithms is on kernel methods such as KCUSUM, NEWMA and Mstats-CPD that will be discussed in detail in Chapter 3.

1.4 Chapter Overview

Below is short description of each chapter and its contents. Ideally, each chapter should be read chronologically, but effort has been made so that each chapter is as self-contained as possible.

Chapter 2 provides a background on hypothesis testing and its relation to the change point detection problem. The online change point problem is formulated along with measures for evaluating performance. The chapter closes out by reviewing classic methods for detecting change points on streaming data.

Chapter 3 examines kernel change point detection as it is a focus of this thesis. A short background on the maximum mean discrepancy and its use in two-sample hypothesis tests is covered first. This is followed by a review of the most competitive online, kernel change point detection methods.

Chapter 4 applies our change point detection algorithm to liquidity in financial markets. A model of the limit order book is presented and the construction of the financial dataset is explained.

Chapter 5 concludes the thesis by summarizing all the results and discussing future avenues for research.

Chapter 2

Background

This chapter describes how the change point problem will be formulated in this thesis and, by extension, how all methods will be described using the change point detection problem notation. Because online change point detection is closely related to two-sample testing, a background on statistical hypothesis testing is presented first.

2.1 Hypothesis Testing

Let x and y be random variables defined on the topological space $\mathcal{X}$ with probability distributions P and Q respectively. Assume we draw n observations from P and m observations from Q resulting in two samples $X = \{x_1, x_2, ..., x_n\} \sim P$ and $Y = \{y_1, y_2, ..., y_m\} \sim Q$, where each sample is independently and identically distributed with respect to P and Q. The main question posed in this thesis is can we determine if P and Q are statistically the same or different distributions.

To answer this question, we use the *statistical hypothesis testing* framework as it is described in [8]. Generally, a *hypothesis* is a statement about a population parameter, θ. Examples of a population parameter are the population mean, variance or other higher order moments. In hypothesis testing, we trying to determine whether one of two complementary hypotheses is true. The first, denoted by H_0, is called the *null hypothesis* and it states that $\theta \in \Theta_0$ where Θ_0 is some subset of the parameter space. The second hypothesis, denoted by H_1, is called the *alternative hypothesis* and it states that $\theta \in \Theta_0^c$. For instance, if it is believed P and Q are distinguishable by

their population means, $\mathbb{E}[P]$ and $\mathbb{E}[Q]$, then the possible hypotheses are:

$$\begin{cases} H_0 : \mathbb{E}[Q] \in \{\mathbb{E}[P]\} & \text{(same mean, i.e. } P = Q) \\ H_1 : \mathbb{E}[Q] \notin \{\mathbb{E}[P]\} & \text{(different mean, i.e. } P \neq Q). \end{cases} \tag{2.1}$$

How do we pick between H_0 and H_1 in equation 2.1? Every hypothesis test relies on a corresponding *test statistic* T that is a real-valued random variable. Because P and Q are unknown in our context, an estimate $\hat{T}$ can be calculated using X and Y such that $T : \mathcal{X}^n \times \mathcal{X}^m \to \mathbb{R}$, which yields:

$$\hat{T} = T(X, Y). \tag{2.2}$$

The test statistic $\hat{T}$ is then compared to some *threshold* selected by the user. There many ways to set such a threshold, but usually if the test statistic exceeds the threshold then H_0 is rejected and H_1 is accepted. Otherwise, the hypothesis test fails to reject H_0.

A common way to set the threshold is through a significance level, $\alpha \in [0,1]$ that is chosen at the outset. Common choices for α are $0.1, 0.05$ and 0.01 [43]. The test statistic is compared to α by computing a *p-value* that is estimated by $\hat{p} = P(T \geq \hat{T}|H_0)$. The p-value is the probability of observing $\hat{T}$ under the null hypothesis. A p-value $< \alpha$ would be improbable under the null hypothesis, therefore, in this situation it is rejected and the alternative hypothesis is accepted.

Given the binary outcome of a two-sample test, it is clear the hypothesis test can fail in the two following ways. The first is rejecting the null hypothesis when it is correct. This is known as a false positive or a type-I error and is upper-bounded by the chosen significance level, α. It is equivalent to following conditional probability: $\mathbb{P}(\text{reject } H_0|H_0 \text{ is true})$. The second possible source of error is a false negative or type-II error. The probability of committing a type-II error is denoted as $\beta = \mathbb{P}(\text{accept } H_0|H_0 \text{ is false})$. The quantity $1 - \beta$ is referred to as the *power* of a test. Maximizing test power is an important part of designing new algorithms and is typically used to compare different methods.

Often there is a trade-off between type-I and type-II errors and the practitioner must decide how to balance the two given their domain-specific knowledge of the problem. In some cases, it may be desirable to sacrifice one for the other. For example, in the medical field [37], a false positive diagnosis (type-I error) may be

more desirable than missing a diagnosis (type-II error) which would result in never giving treatment to a patient.

Note there is not a lot of information at our disposal for constructing a non-parametric two-sample hypothesis test. Distributions P and Q are unknown, X and Y are the observed data and the other settings are chosen according to the specific hypothesis test. This means the main decision left up to the practitioner is determining what statistical test to use. In other words, what T should be used for evaluating equation 2.2? The choice should depend on how P and Q may differ from each other. For example, the Student t-test is a two-sample test for determining if samples of univariate data come from a population with the same mean [58]. A generalization of the Student t-test for the multivariate case is the Hotelling T^2 test that compares whether the means of two multivariate samples are significantly different [25]. Both of these are parametric tests as they assume the samples are normally distributed. This means, in the context of our problem where nothing is known about P and Q, they are not suitable tests for comparing two samples.

Alternatively, non-parametric tests make no assumptions about the distributions P and Q. For example, the Kolmogorov-Smirnov test (KS test) [42] can determine whether or not two univariate samples come from the same distribution. This is done by computing the *supremum* of the difference of the empirical cumulative distribution functions from each sample. The KS test does not specify what distribution the samples come from, only if they differ according to the KS statistic. More recently in [17] , the kernel two-sample test is introduced as a flexible, non-parametric test. It is not limited to one dimensional data, and can be applied to non-numeric data. It is based on the *maximum mean discrepancy* (MMD) statistic and is capable of detecting any kind of change in distribution. It is a focus in this thesis and is discussed in more detail in section 3.1.

2.2   Problem Formulation

Because there is no official standard formulation for the online change point detection problem in the literature, we use the description in [32] as the basis for the following problem description.

2.2.1   Change Point Detection Problem

Consider a data stream X to be a sequence of random variables, $X_1, X_2, X_3, ...$ where each X_t for $t = 0, 1, 2, ...$ is generated by some probability distribution P_t and each X_t is independent of the one that came before it. A change point occurs at time $t+1$ if $P_t \neq P_{t+1}$. The goal of online change point detection is detecting this change point as soon as possible.

Consider the case where we don't know when $P_t \neq P_{t+1}$ and we rely only on the observed values X_t to answer this question. We can re-frame the online change point problem to the problem of comparing two sets from X. The intuition behind this is simple. If indeed a change point occurs then any observed values after the change point should exhibit a statistical difference with observed values prior to the change point. We simply need to decide what observations should be part of each set so that a significant comparison can be made. Using this approach, a general formulation can now be made.

Let w be the number of most recent observations of X. Let this set be denoted by $X_t^w = \{X_{t-w}, ..., X_{t-1}, X_t\}$ whose length is the window, w where $w \in \mathbb{Z}^+$. This recent set will be compared to some reference set of X denoted by $X_t^{ref} = \{X_0, X_1, ..., X_{t-w}\}$ whose distributions $P_0 = P_1 = ... = P_{t-w}$ are sampled from a common distribution P. What is this reference set? It is data that is known to be distributed consistently prior to a change point. In the process control literature, it is known as the in-control distribution [5]. We will use these terms interchangeably as they capture the same idea. We do not explicitly state how many observations are stored for X_t^{ref} because this depends on the change point detection method used.

Let θ_t be the parameter we expect to change in our data stream at a particular time. The most recent parameter θ_t^w will be compared to the set reference parameters, $\{\theta_0, \theta_1, ..., \theta_{t-w}\}$, to determine if a change point has occurred. In other words, at each time, t, the online change point detection problem is performing the following hypothesis test:

$$\begin{cases} H_0 : \theta_t^w \in \{\theta_0, \theta_1, ..., \theta_{t-w}\} & \text{(no change point occured)} \\ H_1 : \theta_t^w \notin \{\theta_0, \theta_1, ..., \theta_{t-w}\} & \text{(a change point occured)} \end{cases} \tag{2.3}$$

If the null hypothesis is true then the streaming data is distributed consistently along P and no change point exists. If the null hypothesis is rejected, the time series may

be partitioned by a change point, t^*, that signifies all data from $t \geq t^*$ are distributed differently than data from $t < t^*$. Because we are operating in a non-parametric setting, the parameters used for comparison are estimated using the streamed data and aren't assumed to follow any particular family of distributions.

Many change point detection algorithms define a statistic that is computed using each set before and after the possible change point [1]. If the statistic is above a threshold, $h \in \mathbb{R}$, then time t is classified as a change point. The estimated change point time is denoted as $\hat{t}$ and can be compared to underlying true change point, t^*, if it is known.

The size of the window, w, is an important consideration that is typically chosen based on the problem being solved. A small window will detect change points more frequently resulting in fast change point detection but at the cost of more incorrect detections. A large window will have the opposite problem. The change point method will have less incorrect detections but will be slower to detect real change points.

2.2.2 Performance Measures

Every time the change point hypothesis test in 2.3 is evaluated two main issues arise. The first is detecting a change point when there is no actual change in the observed sequence. These are typically called *false alarms* or false detections in the change point detection literature [35]. The second issue is not detecting a change point when one occurs, called a *missed detection*. This could be caused by detecting a change point much too late for it to be of any use or simply missing it altogether. In both cases, a running total of false alarms and missed detections is monitored for performance. However, simply counting the number of false alarms or missed detections does not capture the goal of the online change point detection problem, which is to quickly detect change points over time, while minimizing false alarms.

The expected amount of time that must pass before observing a false alarm is defined by a metric known as the *average time to false alarm* (TTFA). It is defined as:

$$\text{TTFA} = \mathbb{E}[\ \hat{t}\ |\ t^* \text{ does not exist}], \tag{2.4}$$

where it is the expected number of observations that are observed before a change point is incorrectly detected. Therefore, a larger value of TTFA is preferable. In the

literature it is also referred to average run length (ARL) or average run length under the null (ARL_0) [29].

The second method of evaluating the accuracy in the context of online change point detection is the *expected detection delay* (EDD). It is the expected amount of time that passes before a true change point is detected. It is defined as

$$\text{EDD} = \mathbb{E}[\ \hat{t}\ |\ t^* \text{ does exists}]. \tag{2.5}$$

An online change point detection technique aims to minimize EDD, while maximizing TTFA. Balancing the two is similar to balancing type-I and type-II error discussed in section 2.1, where the practitioner may one to sacrifice one for the other. A lower EDD will necessarily result in a lower TTFA, which is undesirable.

2.3 Classic Algorithms

Presented below are the fundamental approaches to online change point detection that have been very influential on modern approaches. Many modern algorithms are variants of the classic algorithms discussed below. In the following sections let X_t be defined as it is in 2.2.1.

2.3.1 Shewart Control Chart

Shewart control charts were originally designed to detect changes in the mean of a process where the values being observed are assumed to be Gaussian distributed [54]. As the data arrives, the data is batched into samples of size N. The sample mean, $\bar{X} = \frac{1}{N}\sum_{t=1}^{N} X_t$, is the then calculated and compared it to a known, true mean μ^*. Similarly, it is assumed the standard deviation, σ, is known in advance but it can also be estimated. If the absolute difference is greater than a threshold, then a change point is declared at the current batch. Therefore, the decision rule is defined as,

$$|\bar{X} - \mu^*| > \kappa \frac{\sigma}{\sqrt{N}}, \tag{2.6}$$

where $\kappa \in \mathbb{R}$ is a constant that controls how sensitive the algorithm is. Typically, it is set to $\kappa = 3$ as this coincides with the observations within 3 standard deviations of the mean. Under the assumption that the data is distributed normally, approximately 99.7% of the observations are distributed in this region, therefore a change point is

declared if it falls outside this region. The true mean is assumed to known and is defined as $\mu^* = \mathbb{E}[X_t]$. In applications, the true mean can also be replaced by some target specification that a process must adhere to.

Tuning the hyper-parameters can drastically change the performance of the algorithm. The parameter κ is used to control the trade-off between false alarms and missed detections. Choosing a lower κ makes the control chart detect change points more often and, consequently, increases the false alarms. Whereas a higher κ results in less false detections but also more missed detections. The chosen sample size, N, is also critical and its effect on the performance of Shewart control charts is studied in [21].

2.3.2   CUSUM

Similar to the Shewart control chart, the CUSUM algorithm tracks a statistic over time relative to a predetermined threshold [47]. CUSUM is best applied to a process that is already under control. It can be thought of accumulating the information of current and past samples.

The algorithm is defined by a statistic, $S_t \in \mathbb{R}$, that is recursively updated after each sample, X_t, is observed, such that:

$$
\begin{cases}
S_0 = 0 & \text{(Initialization)} \\
S_t = \max(0, S_{t-1} + Z_t) & \text{for t=1,2,...,}
\end{cases}
\tag{2.7}
$$

where $Z_t = ln(\frac{f_1(X_i)}{f_0(X_i)})$ and the statistic S_t is compared to a threshold $h \in \mathbb{R}$ that is predetermined by the user. Functions f_0 and f_1 are probability density functions for the pre-change distribution and post-change distribution respectively. If $S_t \geq h$ then a change point is declared at time t and the algorithm is either stopped or restarted. Given that the statistic only flags change points when greater than a threshold, this algorithm only detects positive changes in the distribution. In [47], it is suggested to combine two CUSUM algorithms to detect positive and negative changes in a distributional parameter.

As a parametric algorithm, it is assumed f_0 and f_1 are known at the outset. In most applications, this is quite limiting and unrealistic. Therefore, in cases where they are unknown, *maximum likelihood estimates* of each distribution's parameters are usually computed. See [30] for details on maximum likelihood estimation.

Several extensions to the CUSUM algorithm have been proposed such as the filtered-derivative extension introduced in [4], which uses the change of the discrete derivative of a signal over time to detect a change point. In [40], a fast initial response (FIR) CUSUM algorithm is proposed where the starting value of initial cumulative sums adapts over time. Instead of resetting S_0 to zero as shown above, it is reset to a non-zero value, typically based on the threshold chosen. This gives the algorithm a head-start in quickly detecting when a process is out of control and is especially useful for processes that don't start in control.

Finally, since CUSUM is typically better at detecting small shifts in signals and the Shewart control chart is faster at detecting larger changes, the two can be combined [39]. The combined Shewart-CUSUM algorithm leverages the strengths of both techniques for better overall performance. See [64] and [62] for more details.

2.3.3   EWMA

First described in [51] as a *geometric average*, the exponentially weighted moving average (EWMA) is a type of moving average that applies exponential weighting to time series samples. Initially used as a forecasting technique in the econometrics field for smoothing noisy functions, the EWMA can also be used for determining out of control processes as shown in [26]. Rather than weighing all observations uniformly like the standard CUSUM algorithm or a simple moving average, a decay factor (also called a forgetting factor), $\lambda \in [0, 1]$, is used to control how much weight is distributed over the previous observations. As each new observation arrives, the EWMA statistic, $E_t \in \mathbb{R}$, is recursively updated and compared to a threshold. If the EWMA statistic exceeds the threshold then the process is deemed out of control or, in other words, a change point is detected.

The EWMA statistic is calculated as follows at each time step, t:

$$E_t = \lambda X_t + (1 - \lambda)E_{t-1}.$$

As $\lambda \to 1$, the EWMA gives more and more weight to the most recent observations similar to a Shewhart control chart, which gives weight to the last observation only. Conversely, as $\lambda \to 0$, the weights are distributed further into the past giving the EWMA a longer memory similar to the CUSUM algorithm. Therefore, a EWMA control chart can be interpreted as a trade-off between a Shewhart control chart and

a CUSUM control chart.

For detecting deviations away from a mean target value, control limits may be calculated in a similar manner to the Shewart control chart. In [26], control limits for the EWMA are chosen to be $\pm 3\sigma \sqrt{\frac{\lambda}{2-\lambda}}$. Like the Shewart control chart, it is assumed the standard deviation, σ, is known in advance but it can be estimated if it is not known.

As with the other methods previously mentioned, the standard EWMA is a parametric method as it assumes the time series has some in-control average that is known prior to use. This makes is difficult to apply in situations where the data is coming from unknown distributions. It is however very fast due to its recursive structure and does not hold a lot of data in memory making it appealing for live data streams that need fast data processing.

Chapter 3

Kernel Change Point Detection

In this chapter, we focus on the class of change point models that leverage kernel techniques, known as *kernel change point detection*. A unique feature of kernel methods is the use of the maximum mean discrepancy (MMD) metric as the change point test statistic. Therefore, a short review of the MMD statistic is presented first.

3.1   Kernel-Based Test Statistic

Recall we are looking for a suitable statistic to solve the change point hypothesis test presented in 2.3. To solve this, we need a statistic that can measure the difference between two distributions, P and Q. In our setting, this is particularly hard because we do not know P or Q and only have access to data generated by them. Ideally, the metric measuring the difference should return a small value if $P \approx Q$ and large value if P and Q are very different from each other. This means we need a metric that can compute the distance between two probability distributions using only data drawn from them. It turns out the maximum mean discrepancy (MMD) introduced in [17] meets all these criteria.

The idea behind the MMD is the following: rather than comparing the expected value of P and Q in their original feature space, why not compare their expected value in a different feature space that makes discerning between P and Q more effective. Doing so would allow the detection of differences between P and Q that were not possible before. A classic technique for comparing samples in a different feature space is through the use of kernel functions. Therefore, we'll start with a brief background

of kernel functions.

3.1.1 Kernel Background

Suppose we have a non-empty set $\mathcal{X}$ for which $x, y \in \mathcal{X}$. A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a *kernel* if there exists a *feature space* $\mathcal{H}$ with a corresponding *feature map* $\phi : \mathcal{X} \to \mathcal{H}$. A kernel can be expressed as,

$$k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}} \tag{3.1}$$

where $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is the *inner product* in $\mathcal{H}$ [53]. Using the kernel function, we can feed it two points and implicitly compute the dot product of these points in the transformed space. This is the so-called *kernel trick*. It's a trick because the dot product can be computed without having to explicitly know the feature map or what the coordinates of $\phi(x)$ or $\phi(y)$ evaluate to. Lastly, because dot products are symmetric, this implies that the kernel function as defined above is also symmetric, i.e. $k(x, y) = k(y, x)$.

A related concept is the *Gram matrix* which can be computed from a set of vectors $\{\mathbf{x}_1, .., \mathbf{x}_\ell\}$ as an $\ell \times \ell$ matrix $\mathbf{G}$, whose entries are $\mathbf{G}_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$. Using 3.1, we can define a *kernel gram matrix* or just *kernel matrix*, denoted by $\mathbf{K}$, as:

$$\mathbf{K}_{ij} := k(\mathbf{x}_i, \mathbf{x}_j). \tag{3.2}$$

By symmetry of the kernel, the kernel matrix is also symmetric $\mathbf{K}_{ij} = \mathbf{K}_{ji}$ or $\mathbf{K}^{\mathrm{T}} = \mathbf{K}$. More explicitly, it is expressed as:

$$
\begin{array}{c|cccc}
\mathbf{K} & 1 & 2 & \cdots & \ell \\
\hline
1 & k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \cdots & k(\mathbf{x}_1, \mathbf{x}_\ell) \\
2 & k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \cdots & k(\mathbf{x}_2, \mathbf{x}_\ell) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\ell & k(\mathbf{x}_\ell, \mathbf{x}_1) & k(\mathbf{x}_\ell, \mathbf{x}_2) & \cdots & k(\mathbf{x}_\ell, \mathbf{x}_\ell)
\end{array}
\tag{3.3}
$$

In most applications, k is chosen to be positive definite. A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a positive definite kernel if it is symmetric and

$$\sum_{i,j=1}^{n} c_i c_j k(\mathbf{x}_i, \mathbf{x}_j) \geq 0, \tag{3.4}$$

for any $n \in \mathbb{N}$, any choice of $\mathbf{x}_1, ..., \mathbf{x}_n \in \mathcal{X}$ and any $c_1, ..., c_n \in \mathbb{R}$. This is equivalent to requiring that the constructed kernel matrix has entirely positive eigenvalues. Furthermore, there always exists $\phi : \mathcal{X} \to \mathcal{H}$ for which equation 3.1 holds if k is positive definite.

By selecting a positive definite kernel, the feature space $\mathcal{H}$ is actually a space of functions known as a *reproducing kernel Hilbert space* (RKHS). While this may seem odd, it actually simplifies a lot of algebra because elements in a RKHS can be treated like finite vectors. For the purposes of this thesis, we will only deal with positive definite kernels to ensure the corresponding feature space is a RKHS.

3.1.2 Kernel Mean Embedding

While kernel functions are useful for comparing vectors in a new feature space, this is not quite what we need because we are looking for a way to compare two probability distributions. In the above setting, ϕ accepts points or vectors as inputs, but this can be generalized to random variables in the following way: Let X be a random variable with domain Ω and distribution $P(X)$. We refer to instantiations of X as a lower case x. In [55], it is shown that ϕ can be used to represent a probability distribution as an element in a RKHS by

$$\mu_X = \mathop{\mathbb{E}}_{X \sim P}[\phi(X)], \tag{3.5}$$

which is known as the *kernel mean embedding* of P. This can be interpreted as a distribution being mapped to its expected feature map in $\mathcal{H}$.

Because we are in a non-parametric setting, we cannot assume what $P(X)$ is. However, we can estimate the embedding using a finite sample average [55]. Suppose we have access to a sample $\{x_1, x_2, ..., x_m\}$ where x_i is drawn i.i.d from $P(X)$, the empirical kernel mean embedding is

$$\hat{\mu}_X = \frac{1}{m} \sum_{i=1}^{m} \phi(x_i). \tag{3.6}$$

See Figure 2 for a better understanding of the relationship between the distribution, the instances of the random variable and their embeddings into the new feature space.

Figure 2: Stylized depiction of a kernel mean embedding of $P(X)$ to a RKHS as μ_X. The empirical estimate, $\hat{\mu}_X$, is shown to be close in $\mathcal{H}$ to its theoretical counterpart.

$P(X)$ $\mathbb{E}[\phi(X)]$ Feature Space

μ_X

$\hat{\mu}_X$

x_i X

$\phi(x_i)$
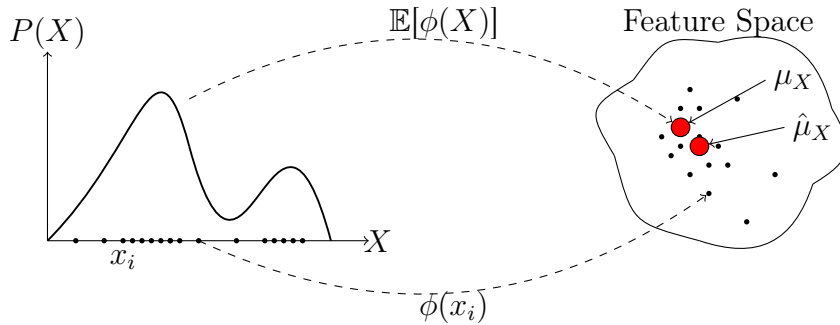
Why bother mapping P to a RKHS? Because we can now compare two probability distributions in $\mathcal{H}$ as if they were vectors in an infinite-dimensional space. This means we can use vector operations such as dot products or norms with kernel mean embeddings.

While this new feature space representation is helpful, it is not necessarily unique. This a problem because P and Q may be mapped into a space where they are measurably similar when in fact they are not. Consequently, we need to ensure the kernel mapping is *injective*, i.e. that the mapping from $\mathcal{X}$ to $\mathcal{H}$ is one to one.

To ensure the kernel mapping is injective, we can make use of a special class of kernel functions known as *characteristic kernels* that are introduced in [14] and [56]. These papers show that if k is characteristic then the mapping of ϕ into the $\mathcal{H}$ is unique. This means if a characteristic kernel is used, then X and Y can be uniquely mapped to another feature space where the expected value in $\mathcal{H}$ is also unique.

With this last piece of information we can now map two different distributions into a new feature space and compute a distance-like metric between the two, which is the basis of the maximum mean discrepancy.

3.1.3 Maximum Mean Discrepancy

Suppose m observations from a sample $\{x_1, x_2, ..., x_m\}$ and n observations from a different sample $\{y_1, y_2, ..., y_n\}$ are derived from $\mathcal{X}$. Assume the observations from each sample are instantiations of random variables $X \sim P$ and $Y \sim Q$ respectively. Using ϕ as it is described in 3.1, the maximum mean discrepancy (MMD) is defined

in [55] as:

$$\text{MMD}(P,Q) = ||\mu_X - \mu_Y|| = ||\underset{X \sim P}{\mathbb{E}}[\phi(X)] - \underset{Y \sim Q}{\mathbb{E}}[\phi(Y)]||_{\mathcal{H}}, \qquad (3.7)$$

where $|| \cdot ||_{\mathcal{H}}$ is the *norm* on $\mathcal{H}$. The MMD can be interpreted as the distance in $\mathcal{H}$ between the kernel mean embeddings of the features. As long as a kernel function can be defined on the given data structure, the MMD can be used. This is why it can be applied to non-numeric data such as strings, graphs, and other structured domains [24]. From theorem 5 of [17], the theoretical $\text{MMD}(P,Q) = 0$ if and only if $P = Q$. This fact arises from the injective property defined earlier. While this is a nice property, in practice we use empirical estimates of the kernel mean embeddings, $\hat{\mu}_X$ and $\hat{\mu}_Y$, meaning an estimate of MMD will never be exactly zero even if our samples are from the same distribution. Nonetheless, the power of MMD lies in its ease of estimation and the fact that it can detect any type of parameter difference between P and Q.

Using X and Y, the unbiased estimate of the squared MMD is shown in [17] to be:

$$\widehat{\text{MMD}}_u^2(X,Y) = \frac{1}{m(m-1)} \sum_{i=1}^m \sum_{j=1}^m k(x_i, x_j) - \frac{2}{mn} \sum_{i=1}^m \sum_{j=1}^n k(x_i, y_j) +$$
$$\frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j=1}^n k(y_i, y_j). \qquad (3.8)$$

One caveat of equation 3.8 is that while it is an unbiased estimate of the square of 3.7, the calculation of $\sqrt{\widehat{\text{MMD}}_u^2}$ is not an unbiased estimate of 3.7.

Similarly, the biased estimate of the squared MMD is

$$\widehat{\text{MMD}}_b^2(X,Y) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(x_i, x_j) + \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m k(y_i, y_j) - \frac{2}{nm} \sum_{i=1}^n \sum_{j=1}^m k(x_i, y_j). \qquad (3.9)$$

Because both 3.8 and 3.9 are computed in $\mathcal{O}((m+n)^2)$ time, they will be referred to as quadratic-time estimates of MMD. For high-dimensional datasets (large m or n), using a quadratic-time estimate of MMD is impractical.

An alternative is proposed in section 6 of [17] that is linear in computation time and still uses all available data. Letting X and Y have equal size m for notational simplicity, then

$$\widehat{\text{MMD}}_l^2(X,Y) := \frac{1}{m_2} \sum_{i=1}^{m_2} h((x_{2i-1}, y_{2i-1}), (x_{2i}, y_{2i})) \qquad (3.10)$$

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is the linear-time estimate of MMD, where $m_2 = \frac{m}{2}$ and

$$h\left((x_i, x_j), (y_i, y_j)\right) := k\left(x_i, x_j\right) + k\left(y_i, y_j\right) - k\left(x_i, y_j\right) - k\left(x_j, y_i\right). \tag{3.11}$$

This estimation of the squared MMD is computed in $\mathcal{O}(m)$, which is significantly faster than the quadratic-time estimates. However, it pays for this speed with accuracy as the MMD_l estimate has higher variance than MMD_u.

Now that we have a suitable metric for computing a test statistic between samples X and Y, a hypothesis test can be constructed using the MMD statistic as shown in [17]. Similar to previous hypothesis tests, a threshold and kernel function is chosen to adequately balance between type-I and type-II error. The null hypothesis is that X and Y are equivalent in their kernel mean elements. If the MMD is greater than the threshold, then the null hypothesis is rejected and the alternative hypothesis is accepted. In this case, the alternative hypothesis would indicate X and Y differ in one or more of their statistical moments.

3.1.4   Choice of Kernel

Notice we have not yet explicitly chosen a kernel function for calculating the MMD statistic. Choosing the proper kernel is often done on a per case basis. Overall optimal kernel selection is a difficult problem that is still actively researched [13] [19]. We will only discuss one kernel function in this thesis, the Gaussian kernel. The Gaussian kernel is the most widely used kernel and it is the only kernel used in the kernel change point detection methods discussed in section 3.2. For other possible choices of kernel functions see table 3.1 in [45].

Given two d dimensional real vectors $x, y \in \mathbb{R}^d$, the Gaussian kernel is defined as:

$$k(x, y) = e^{-\frac{1}{2\sigma^2}||x-y||^2} \tag{3.12}$$

where $\sigma > 0$ and is called the *kernel bandwidth*. In [18], the authors recommend selecting the bandwidth based on the *median heuristic*, which computes σ according to,

$$\sigma = \text{median}\{||x_i - x_j|| : i, j = 1, ..., n\}, \tag{3.13}$$

which is the median of the pairwise distances between data points. It is not clear where this heuristic was first introduced although many papers incorrectly cite [53].

Despite its unknown origins, it has been shown to be empirically suitable for many kernel applications. In [15], a large sample analysis of the median heuristic was done to expand what little theoretical understanding there is of it. However, it has been shown to be sub-optimal in high-dimensional and small-sample cases as shown in [44] and [50].

It seems as long as the bandwidth is chosen $\mathcal{O}(\sqrt{\lceil})$ then test power is independent of the bandwidth. It is interesting to note such a critical hyperparameter for performance is tuned heuristically.

Despite this, the median heuristic remains extremely useful for selecting the bandwidth hyperparameter. It is noteworthy then to see how online change point models tune median heuristic. In the context of an infinite data stream, you can simply run and expanding median on all incoming data that infinitely grows. But is this ideal? This would require storing all the observations you ever observe which is obviously intractable. Alternatively, you can set it using some initial training data but again how long is an initial bandwidth valid in a continuous data stream? To our knowledge, these questions have not been addressed anywhere in the kernel change point detection literature, which is why the topic successive median calculation is a focus in section 3.3.

3.2   Related Work

3.2.1   Offline Kernel Change Point Detection

While offline change point detection techniques are not the focus of this thesis, we provide a short summary of some kernel approaches in this domain to highlight some commonalities with online kernel approaches.

There are several common characteristic that offline kernel change point detection have with online kernel CPD. The first of data for which a kernel can properly reproduce a Hilbert space and thereby make use of the MMD statistic. The second is that all offline kernel change point methods cited here make use of the Gaussian kernel, which speaks to the ubiquitousness of this kernel function.

In [20], the authors approached the offline change point problem with a fixed number of change points using kernel change point detection. This was further extended to an unknown number of change points in [2]. The authors show their kernel change

point detection procedure outputs an offline segmentation near optimal with high probability. The authors recommend choosing the kernel based on best possible signal to noise ratio. Therefore, they rely on prior knowledge of a reference or training set is necessary for calibrating the kernel.

More recently in [9], a kernel change point detection method is proposed that uses deep generative models to augment the test power of the kernel two sample test statistic. They point out MMD's lack of test power when using small samples from the out of control distribution, which may easily leading to over-fitting with kernels. Thus, they use a generative adversarial neural network (GAN), trained on historical samples of $X \sim P$ with noise injected into X. This surrogate distribution is then used in conjunction with possible change points to improve the test power of a modified MMD measure that makes use of compositional kernels. The method is compared to other prominent change point methods for offline change detection. All comparisons are done on synthetic data with piece-wise i.i.d. data. All methods are benchmarked using the AUC metric for classification performance and it is shown the KL-CPD method is competitive or better than the state of the art methods. Furthermore, the AUC performance is maintained as the dimensionality of the data is increased, making their kernel learning framework very interesting for future off-line change point detection. It remains to be seen if this framework can be adopted in an online context where time to detection is a key constraint on practicality.

See section 4.2.3 in [61] for a review of kernel-based methods used for offline detecion.

3.2.2   Online Kernel Change Point Detection

One of the first papers to use the term kernel change point detection was in [11]. The authors present an online kernel change point detection model based on single class support vector machines (ν-SVMs). They train two single class support vectors, one on a past set and one on a future set. A ratio is then computed between the two sets that acts as the dissimilarity measure in a Hilbert space. If the sets are sufficiently dissimilar over some predetermined threshold, then a change point is assigned to the time step that splits the two sets of data. The authors argue that a dissimilarity measure between kernel projection of points in a Hilbert space should estimate the *density supports* rather than estimate the probability distributions of each set of

points. While this approach inspired a lot of interesting research that will be discussed below, it does not use the maximum mean discrepancy and has not been studied since.

The following methods are all inspired by the classic algorithms from section 2.3. They all make use of a variation of the maximum mean discrepancy. They are also the most recent online kernel techniques developed and will be used for experiments in later sections. Thus, they will be described in more detail than previous methods.

In [36], the authors use the B-test introduced in [65] and develop an offline and online change point detection algorithm called the MStats algorithm (the authors also refer to this algorithm as the Scan-B algorithm in a follow-up paper). At each time-step, the online model samples new data from a window of size B_0 and computes a B-test statistic with N past samples that are kept as reference samples.

$$Z_{B_0,t} := \frac{1}{N} \sum_{i=1}^{N} \mathrm{MMD}_u^2 \left(X_i^{(B_0,t)}, Y^{(B_0,t)} \right) \qquad (3.14)$$

The resulting test statistic is then normalized by $Z_{B_0,t}/\sqrt{Var[Z_{B_0}]}$ where the authors provide a theoretical calculation of $\mathrm{Var}[Z_B]$. If the normalized test statistic exceeds some predefined threshold then a change point is declared. The B-test is memoryless in the sense that the statistic is calculated each time and only the value of the last calculation has any weight. This is similar to a Shewart control chart that calculates a z-score at each iteration. Adjusting the size of the window, B_0, results in the usual trade-off of performance in online change point detection. A smaller block size will have a smaller computational cost and a smaller detection delay but will result in higher type II error. A larger block size will have better type II error but will take longer to compute. Unfortunately, no matter what block size is chosen, the computation time for the Scan-B algorithm is the longest relative to the other kernel change point methods discussed below.

From here, theoretical bounds are developed for the time to false alarm rate and expected detection delay. They run several experiments on synthetic data including change in mean, change in variance, change from Gaussian to Gaussian mixture, and change from Gaussian to Laplace distribution. Experiments are also done on real-data sets including a speech dataset and the Human Activity Sensing Consortium (HASC) dataset where the performance was better than the relative density-ratio (RDR) algorithm described in [38].

A modified, "no-prior-knowledge" exponentially-weighted moving average called

NEWMA is introduced in [31]. Based on the standard exponentially weighted moving average shown in 2.3.3, NEWMA computes two EWMA statistics of different weights. If the difference between the two EWMA statistics exceeds a predefined threshold then a changepoint is declared at that time step. The reason for using two EWMA statistics is to set one to have a larger forgetting factor. Any recent changes in a distribution will weigh heavily on one statistic, resulting in a sudden, large difference between the two statistics.

Since a standard EWMA is a parametric method, the authors apply a kernel mapping function, Ψ, to the data prior to applying the exponential weights. This provides a memoryless, non-parametric, online change point detection method that does not need to constantly store all previously streamed data. Once the statistics are updated at each iteration, the raw data may be discarded. This characteristic makes it especially useful in applications where security is a concern.

While kernel mean embeddings could be used for approximating, Ψ, as is the case for standard implementations of MMD, this would require the storage of past examples of data. Because the authors aim to reduce run-time cost and storage cost, they use a *random fourier features* (RFF) approach for estimating Ψ (Note RFF is sometimes referred to as *random kitchen sinks*). Because Ψ is estimated using RFF, this is the only method discussed that does not use the kernel function for an implicit representation of the data in another feature. Instead, the RFF explicitly maps the data to a lower dimension Euclidean product space using a randomized feature map $\mathbf{z} : \mathbb{R}^d \rightarrow \mathbb{R}^m$ such that:

$$k(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle_{\mathcal{H}} \approx \mathbf{z}(\mathbf{x})^\top \mathbf{z}(\mathbf{y}) \tag{3.15}$$

where $\mathbf{z}(\mathbf{x}) := \mathbf{W}^\top \mathbf{x}$. Each element, w_{ij}, is sampled from a distribution that is the Fourier transform of a translation invariant kernel [49].

There are several approaches available for calculating RFF already studied in the literature and the authors use three common ones for comparison. They use the standard RFF implementation from [49], the FastFood implementation introduced in [34], and Optical Processing Unit implementation from [52]. All three are used to create three variants of their NEWMA algorithm.

The NEWMA variants are compared to the MStats (Scan-B) algorithm by running empirical experiments on synthetic and real datasets. The synthetic datasets are run using streaming data that is generated from different Gaussian mixture models. They

use an audio dataset for testing on real data. The variants of NEWMA are similar, if not better than MStats (Scan-B) in terms of missed detection percentage. In terms of average detection delay and false alarm trade-off, the NEWMA algorithm and its variants appear to be mildly better as well. The largest advantage of the NEWMA variants over the MStats (Scan-B) method is in the execution time. MStats (Scan-B)'s execution scales linearly with window size, while NEWMA's execution time does not depend on window size.

Finally, in a recent, preprint paper [12], a kernel CUSUM (KCUSUM) algorithm is proposed, where the classic CUSUM algorithm from 2.3.2 is adapted using the faster MMD_l statistic for online detection. The algorithm functions as follows, every two observations, the MMD_l is calculated using newly observed data points and data points sampled from some reference distribution that is known at the outset. The calculated MMD_l acts as the update term to the cumulative sum statistic. If this kernel cumulative sum statistic exceeds some predefined threshold, then a change point is flagged. Interestingly, unlike the previous methods that set the Gaussian kernel's bandwidth using the median heuristic, the authors chose to fix the bandwidth to one. Furthermore, because it relies on a reference distribution that is outside the data stream for comparison, making KCUSUM more of a semi-supervised algorithm rather than a completely unsupervised one.

Besides its speed of computation, an additional benefit of MMD_l is that it is normally distributed under the null distribution unlike the quadratic-time estimate. This facilitates analysis and provides statistical guarantees for worst-case detection delays and the expected time to false alarm. While this non-parametric approach can detect any change in the distribution of a sequence, it does struggle with more complicated distributional changes such as variance changes of a single dimension and changes beyond first and second-order moments. It was also not benchmarked against other kernel methods, which we cover in this thesis for completeness.

3.3   Our Approach

As stated in the related work, all kernel change point detection methods that use a Gaussian kernel use the median heuristic to determine the bandwidth. While this method has proved to be sufficient for most applications, it has not been thoroughly

tested against alternative bandwidth selection procedures. This is ironic given how much impact the choice of bandwidth can have. We present a natural alternative for calculating the median heuristic in real-time for online change point detection. This method is largely based on the `Binapprox` algorithm from [60] that is shown below.

Algorithm 1: Binapprox algorithm

Input: $x_i, .., x_n, B$

Output: Approx. median

Calculate $\bar{x}$ and s_x

Form B bins across $[\bar{x} - s_x, \bar{x} + s_x]$

Map $x_i, .., x_n$ to bins

for *While condition* **do**

    instructions;

    if *condition* **then**

        instructions1;

        instructions2;

$$n(i) = \frac{a}{b(i)\sqrt{3v}}$$

    else

        Return the midpoint of bin b;

    end

end

Several characteristics make `Binapprox` particularly appealing for online, non-parametric data streaming. Firstly, the runtime of `Binapprox` does not depend on a data's distribution. Secondly, the algorithm requires $\mathcal{O}(1)$ storage space, and doesn't perturb the input data, so rearranging is never a problem. Thirdly, in the worst-case scenario the algorithm has $\mathcal{O}(n)$ computational complexity. In practice, it consistently runs faster than the classic quickselect algorithm and `Binmedian`, a more exhaustive algorithm that is presented in the same paper. Lastly, it can handle newly acquired data very quickly to provide an updated approximation of the median.

The main drawback of the algorithm is hinted in its name. It is an approximation of the median and will be at most σ/B away from the true median. Therefore, if the standard deviation of the data is extremely large, the approximation could be significantly different from the actual median. To combat this, the author recommends

setting $B = 1000$, which yields sufficient approximations in most empirical cases.

Naturally, this fits in exactly to what we want to accomplish with online change point detection. We have incoming data that we want to roll into the calculation of the median heuristic but we also want a fast way to update the median while being accurate. The `Binapprox` algorithm checks all of these boxes and is simple to incorporate into any online change point detection work flow.

3.4   Experiment Setup

3.4.1   Initialization

An important factor for online change point methods is determining how to initialize the algorithm. Because we are running an unsupervised model for classifying change points, we do not spend time training the model or tuning any of the hyperparameters. This is a double-edged sword because on one hand, we can drop in a change point algorithm onto a data stream let it start running without much configuration. On the other hand, if it does not have any prior distribution to compare to then it will need to be adjusted to know what's an appropriate reference or in-control distribution. This is usually referred to as the initialization phase for online algorithms.

There are many ways to get through the initialization step and create an appropriate reference sample. One way is to initially compare the oncoming data stream with some zero valued data. As data comes in, the algorithm can replace the reference data with real observations, creating a reference distribution. While this does assume that the data is initially in-control, it does provide a simple way to create a reference distribution on the fly without prior knowledge. When analysing the results, the practitioner must exclude the initial phase when comparisons were done with the initial zero values because the test statistic calculated from them will be insignificant.

Another method is to construct the reference distribution with past data that do not contain change points if it is available as done in [36] and [12]. This method benefits from not having to spend time initializing the algorithm since it can immediately provide an informed statistical comparison. If the data stream is not very long or costly to acquire then this method is beneficial because the entire signal is retained. On the other hand, prior work needs to be done to construct this sample and this may not always be feasible in practice. Another possible issue is what if the regime of the

in-control distribution shifts to a new normal? Then the old reference distribution is no longer applicable and must be recreated again, which may be costly.

3.4.2 Structuring the Data Stream

In practice, there is no universal way for evaluating online change point models given the nature of the problem. There are two main reasons for this. First, because change point detection originated in the statistical literature, most algorithms or models have strong theoretical results but have not being applied to synthetic or real datasets. Being able to handle high dimensional data streams is a relatively new benefit that has not been so research up until the mid-90's was largely theoretical in nature. Second, it's not obvious how an infinite data stream should be simulated to evaluate the efficacy of an algorithm. How long does synthetic data stream have to be to objectively evaluate an algorithm? How can you actually know where change points occurred in a real dataset that has no obvious ground truth? It is not obvious how to answer these questions, nor does there exist a universal answer. Like most things, the answer depends on the context and what a practitioner is aiming to test with their particular algorithm.

For this thesis, we wish to compare several methods not just one novel method, therefore data consistency and reproducibility will be important for drawing conclusions about performance. Synthetic datasets are a good way to replicate different distributions over and over. Real change points can also be exactly identifiable and compared to with synthetic data. Take for example a data stream where a single random variable is sampled from a normal distribution $\mathcal{N}(0,1)$ that incurs a change point and becomes a random variable from a normal $\mathcal{N}(0,2)$. I can control both of these distributions and know exactly where the change point occurred, but how should I determine how many observations should be observed before switching distributions? How many observations after the change point should I draw from the new distribution before realizing the algorithm will never detect this change point? Again, decisions like this are arbitrary and nuanced for evaluating online change point models because there is no universal method.

We choose to

3.4.3 Evaluation

In cases where a change point is detected, the average detection delay (ADD) is used to estimate the average time it takes for a change point to be detected. It is computed by comparing the time difference between a predicted change point and an actual change point. This difference is then normalized the total by the total number of change points:

$$\text{ADD} = \frac{\sum_i^{\#CP} |\hat{t}_i - t^*|}{\#CP} \tag{3.16}$$

The closer the predicted change points are to the actual change points, the smaller the average detection delay. Because it relies on ground truth change points, it can only be used when experimenting on synthetic data where all the information is available.

If labelled change points are available for a real world dataset or a synthetic dataset, then the ground truth change point vector, t^*, is known. Evaluating performance in this case is the same as evaluating a binary classifier from a supervised learning problem. For example, the metrics from discussed in hypothesis testing, type-I error (false positives) and type-II error (false negatives), are commonly used for evaluating change point detection performance. The false positive rate (FPR) can be calculated by $FPR = FP/N$. Plotting the false positive rate and the true positive rate, gives the receiver operator characteristic curve. The area under this curve (AUC), is calculated and compared to random baseline performance of 0.5 that would be equivalent to classification by tossing a coin.

3.4.4 Synthetic Datasets

A common difficulty in change point detection is evaluating the performance of an algorithm with datasets that aren't overly simplistic and difficult enough to ascertain some real world use.

Unlike fields like image recognition where datasets like MNIST provide a common benchmark, there are no standard datasets that are widely used across the change point detection literature for evaluating new methods. Most papers propose experiments that are relevant for the specific problem they are trying to solve but lack examples or explanations of when their method would not be applicable. Furthermore, because change point evolved out of the statistics literature, many papers focus on theoretical results and provide minor experimental results, if any.

Given the empirical focus of this thesis, we attempt to put together the most comprehensive experiments using synthetic data. To the best of our knowledge, no change point detection paper covers as many variations as presented in this thesis. While synthetic datasets are idealistic in their formulation, they provide a good starting point for comparing different methods because many variables can be controlled for. Often in the real world, the exact location of change points is not known. Therefore, it is important for the evaluation of a change point detection algorithm that it performs competitively on synthetic data.

Inspired by recent papers [9] and [12] that attempt to bridge the gap between the statistics and machine-learning literature, the following synthetic datasets are created: change in mean, scaling variance, alternating between a Gaussian distribution and a Gaussian mixture, alternating between Gaussian mixtures, and alternating between Gaussian distribution and Laplace distribution. It is truly hard to properly generalize all the possible situations a non-parametric algorithm may be used in, but the synthetic cases presented in this thesis are common across domains and cover a range of applications.

For a change in mean, a change point is inserted in the time series at some random time where the mean is shifted either positively or negatively. There are two variants to this scenario. In the first, the mean change is in all dimensions simultaneously. In the second variation, the mean change is in only one dimension making it harder to detect.

In the last scenario, the time series alternates from a Gaussian with $\mathcal{N}(0,1)$ to a Laplace distribution with zero mean and unit variance. The idea for this scenario is detecting changes when a data stream is consistent in its mean and variance, but not in its later moments.

For each experiment above, a synthetic time series is created with 500 change points that will be fed into the algorithm. Once the detection statistics are calculated, the evaluation metrics from 3.4.3 are computed. A Monte-Carlo approach is used to estimate false alarm rates and average detection delay at various thresholds.

It should be noted this testing setup is nearly identical to the testing procedure used in the NEWMA except we use longer time series with more change points. The other two kernel algorithms, Scan-B and KCUSUM, did not use long time series with several change points but rather a repeated test approach with a single change point.

Table 1: Synthetic Datasets Summary

Type of Change	No. of Dimensions	Length	No. of Changepoints
Mean (all dimensions)	20	5000	50
Mean (single dimension)	20	5000	50
Variance	20	5000	50
Frequency	1	5000	50
Correlation	2	5000	50
Blobs	10	10 000	50
GMMs	50	10 000	50

Chapter 4

Application to Market Liquidity

In finance, *market liquidity* describes how quickly a market participant may buy or sell an asset without causing significant fluctuations in the price. In liquid markets, there is minimal impact to the price by quickly buying (selling) it. In illiquid markets, a purchase (sale) of the asset will cause the price to rise (fall) resulting in adverse price selection if the buyer (seller) is making a large transaction. In both cases, market liquidity is in constant fluctuation. It is this fluctuation that is the focus of this thesis. By detecting changes in market liquidity a market participant can identify periods of when trading may be more or less favourable. For example, an institutional investor wishing to unwind a large position over the course of several days may want to quickly detect rapid changes in a liquidity that could negatively impact their execution strategy. The following description of the limit order book is based on the notation used in [16].

4.1 Properties of the Limit Order Book

All modern financial markets are set-up as a double-sided auction between buyers (bid side) and the sellers (ask side) called limit order books (LOBs). A market participant may post orders at specific prices on either side of the book. A limit order, denoted by x, is defined as a tuple containing a price, p_x, and a size, w_x where $|w_x| > 0$:

$$x = \langle p_x, w_x \rangle. \tag{4.1}$$

A limit order's size indicates how many units of an asset a buyer (seller) is willing

to trade at p_x. The prices for which an order can be submitted at are discrete prices.

The LOB at time, t, is denoted as $\mathcal{L}(t)$, and it represents the set of all orders currently active at time t. All bid orders are at the best bid price or lower. The best bid price at time, t, is denoted as:

$$b(t) = \max_{\{x \in \mathcal{L}(t) | w_x < 0\}} p_x \tag{4.2}$$

All ask orders are placed at the best ask price or higher. The best ask price at time, t, is denoted as:

$$a(t) = \min_{\{x \in \mathcal{L}(t) | w_x > 0\}} p_x \tag{4.3}$$

The *bid-ask spread* or simply the spread at a time, t, is defined as:

$$s(t) = a(t) - b(t) \tag{4.4}$$

The normalized spread, $s_n(t) \geq 0$, can be defined by:

$$s_n(t) = \frac{s(t)}{\pi} - 1 \tag{4.5}$$

There are many types of orders that can be placed in the LOB. In this context, we assume all orders in the LOB at a given time are basic limit orders. That is, they are orders placed at a specific price with a specific size. Therefore, at a price, p, and a time, t, the total number of orders is:

$$n^b(p, t) = \sum_{\{x \in \mathcal{L}(t) | w_x < 0, p_x = p\}} |w_x| \tag{4.6}$$

On the ask side, it is similarly defined as:

$$n^a(p, t) = \sum_{\{x \in \mathcal{L}(t) | w_x > 0, p_x = p\}} w_x \tag{4.7}$$

Everytime a trade occurs or a resting limit order is cancelled at that price, size is removed from the LOB at that price. If the size at the $b(t)$ reaches zero then the spread increases the $b(t)$ decreases.

Every LOB has two configuration parameters: the tick size, $\pi > 0$, which is the smallest possible price increment between orders at different prices and lot size, which dictates the smallest amount that can be traded. As mentioned in [16], LOB

is essentially a one-dimensional lattice where the dimension is price and every point on the price axis is a multiple [1] of π.

There are two possible distributional changes that are of interest. The first is how the entire distribution of liquidity changes over time. These changes are often associated with events happening in the market such as the start of U.S. trading hours, the release of economic data or a planned speech by the head of the federal reserve. There may also be unplanned events that affect the overall liquidity in the book such as a the 9/11 terrorist attack or a virus outbreak like the Corona virus.
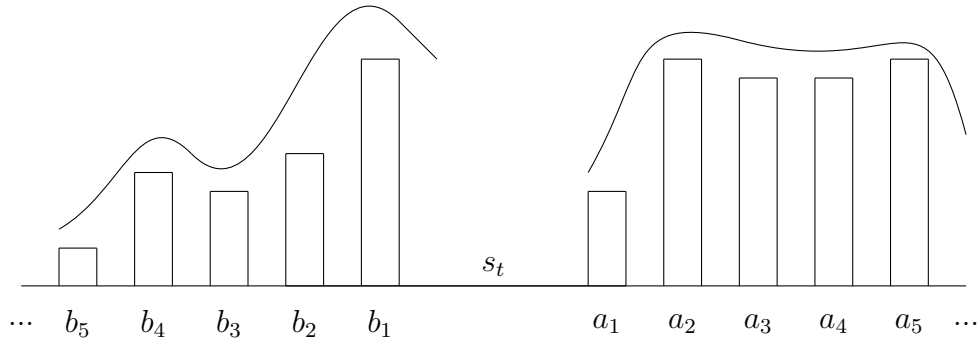
The second is how the distribution of the bid orders differs from the distribution of the ask orders. Typically, the distribution of liquidity on each side of the book is more or less symmetric. However, there have been studies that have shown times when there is an asymmetry between the two sides. This asymmetry has been shown to correlate to price changes.

4.2 Dataset Construction

While many types of markets operate using a basic order book, this thesis will be focused on futures markets found in the Chicago Mercantile Exchange (CME). The reasoning for this is two-fold. The first, unlike bond markets or currency pair markets, liquidity for many futures products is concentrated on a single exchange. This simplifies analysis of liquidity by not having to aggregate data across several exchanges into a synthetic ladder. The second advantage is, unlike equity markets where stocks and exchange traded funds (ETFs) are traded, there are no dark pools available for

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[1]In most cases these multiples of π are strictly positive but in particular markets, such as ED packs and bundles, there may be negative integers of π, i.e. a price axis with positive and negative prices.

the futures markets under consideration in this thesis. Again this simplifies where the liquidity data for an instrument may appear.

The futures that will be used in our dataset are based on a combination of selecting the most traded contracts on the CME and selecting futures that represent different asset classes. They are summarized in the following table:

Table 2: Summary of Futures Studied

Name	Asset Class	CME Symbol	Tick Size	Other
E-mini S&P 500	Equity	ES	0.25	1.402
10 Year T-Notes	Fixed Income	ZN	3.442	0.299
Crude Oil	Commodity	CL	3.442	0.299
Gold	Commodity	GC	3.442	0.299
Euro FX	Currency	6E	3.442	0.299

For each future contract in table 2, the state of the order book is sampled every 60 seconds from 7 AM to 4 PM EST for a period of 45 days. The characteristics of the order book that are sampled at every time step, t_I, are: 1) Quantity, q, at the top N levels of the book, $q_1...q_N$ 2) Spread, $s : [0, \mathbb{Z}^+]$, normalized by tick size, where spread of zero indicates there is no spread.

While spread is not indicative of liquidity but rather an absence of liquidity, we believe it is an important feature to include because all other things being equal, a change in spread is an important change in liquidity distribution for market participants.

Chapter 5

Conclusion

5.1 Summary of the thesis

Add description of thesis, summarizing the key points from each chapter and what this thesis attempted to add to the literature.

5.2 Discussion and Future Work

One focus of this thesis was using the MMD measure for two-sample testing and, by extension, for change point detection. It would interesting to explore other statistical distances that could compare two distributions non-parametrically. It would be interesting to re-use the same approaches explored in this thesis, but with the MMD swapped for a different distance measure.

Recently, interesting research has been made on re-purposing binary classifiers as two-sample tests. In [23], random forests are compared to different implementations of MMD. The authors run many tests comparing the test power across the different two-sample tests and their random forest. The results are interesting because while the random forest classifier is not better in every situation, it is better on hard two-sample tests such as the blobs dataset. Therefore, it remains to be seen whether these classifier approaches to two-sample testing can be adapted to online change point detection in an efficient manner.

- lopez paper

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