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ANALYSIS OF MULTIPLE CHANGE-POINTS IN NORMALLY DISTRIBUTED SERIES.

Por

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Abstract

This research is composed for two researches which abstracts are:

Paper 1: Change-Point Estimation for a Sequence of Normal Observations and Integration with Q-Charts.

This is the first research regarding to change-point analysis for independent observations normally distributed. It considers the case when a single step change has occurred and distribution's parameters (before and after change) are unknown. Development of maximum likelihood estimators (MLEs) for the change-point and parameters is the main concern as well as an integration with control charts in order to show its application in practice, with which retrospective and on-line analysis are both covered. A change is considered as one of the three different cases: (1) change only in mean parameter, (2) change only in variance parameter or (3) change in both parameters. Due to there are change-point estimators for change in mean and change in variance, comparison is done to show what estimator is recommended to use in each situation.

Paper 2: Estimation of multiple change-points in time series normally distributed using a construction Heuristic and a Genetic Algorithm.

This is the second research related to change-point analysis for independent observations normally distributed. It considers case when multiple step changes have occurred assuming that distribution's parameters as well as change-point positions are unknown. Maximum Likelihood estimators for change-points as well as for parameters were developed considering three cases based on single step change problem: (1) multiple changes only in the mean, (2) multiple changes only in variance and (3) multiple changes in both parameters at the same time. Obtaining these change-points MLEs could be considered as an optimization problem, so a Construction Heuristic and a Genetic Algorithm (Evolutionary) were developed based on them. Comparison between these estimators was done in order to show their performance.

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CHAPTER 1. INTRODUCTION TO RESEARCH.

1.1 History and Background.

Every process has variation, which could be left to a chance or be attributed to assignable causes. According to Shewhart's (1931) third postulate assignable causes must be found and eliminated in order to secure a statistical control state: This provides advantages such as reduction in the cost of inspection and the cost of rejection. Thus, this way of management has two aspects: first, the detection of special causes of variation and second finding and eliminating these to bring the process back to control. As soon as the assignable causes are detected, the process will improve. Several tools and procedures have been developed in order to assist in the management of systems; one of the best known tools are control charts that are capable of determining whether or not the process is in statistical control. Nevertheless, when sustained changes have occurred, most of control charts are not able to determine the initial moment of the change, which provoke delays in the application of corrective actions. Change-point analysis is the study of structural changes in series of observations. The problem of estimating the moment of a change is called the change-point problem. Several control charts and change-point estimators have been created by assuming a priori knowledge of distribution parameters while, in practice, this assumption is not always met. In consequence, it seems reasonable to develop such tools.

Control charts were first developed by Shewhart (1931) to determine whether or not variability could be left to chance or common causes. Since then, several control charts have been developed keeping the same objective. Control limits are calculated based on rules provided by the control chart itself, then data or a transformation is plotted with corresponding control limits. If one or more observations fall outside control limits, the chart is said to signal the presence of a potential change in the process and as a consequence, variation could be attributed to special causes, otherwise process' variation is left to chance.

There are two types of changes: isolated, which is an output that could be considered as an outlier because it is the only observation falling outside control limits while others falls

within them, and sustained, which is considered a change in the process distribution characteristics over the next outputs. As it was mentioned, control charts are not usually capable of estimating (estimation is always positively biased) the initial moment when a sustained change occurs. For instance, Figure 1 shows a shift in the mean at 50th observation while the chart detects it until 73rd observation. This delay represents a problem for managers because this signal is away from the real moment of the change and the process' improvement might be retarded which means misspending resources.



Figure 1 Control charts for a time series with a change in the mean. (Chart created using Minitabtm).

The search of initial moment of a change is called change-point problem, and it was first defined by Girshick and Rubin (1952) from a Bayesian approach. Since then, different change-point estimators were found in literature where authors commonly assume prior knowledge of initial parameters. For instance, Hinkley (1970) who was the first in using Maximum Likelihood Method to derive change-point estimators for normally distributed observations with a shift in the mean and for changes only in variance of normal process Samuel, Pignatiello, and Calvin (1998b) developed the change-point MLE. Later, Hawkins

and Zamba (2005a) developed a change-point estimator with no assumption of prior knowledge of parameters using a statistic based on Bartlett's test. Recently, Amiri and Allahyari (2011) catalogued changes in the following 4 categories: single step changes, multiple step changes, changes with linear trend, and monotonic changes; they are presented in Figure 2.



Figure 2. Types of changes studied in CPA. Image obtained from Amiri and Allahyari (2011).

Other problem that was addressed is the case of multiple change points for which Perry, Pignatiello, and Simpson (2007, p.328) proposed that "... this type of behavior might occur as a result of one influential process input variable changing several times, or several influential process input variables changing at different times". Jann (2000) addressed this problem by developing a genetic algorithm based on the t-test but using a cost function in order to determine the number and locations of the change-points of normally distributed independent observations with shifts in the mean.

Since the knowledge of time when the change occurred might boost an improvement process and reduce the cost of rework, waste and downtime, this research aims to develop change-point estimators without assuming prior knowledge about parameters before and after sustained changes occurred using the Maximum Likelihood Method. In addition, estimators for cases where more than one sustained change occurred in mean and/or variance of normal processes will be derivate in order to assess the problem defined by Perry et al. (2007).

1.2 Problem Statement.

Shewhart's Third Postulate for Control states that assignable causes of variation may be identified and therefore eliminated, which is desirable to maintain a state of control (Shewhart, 1931). The following two major advantages are obtained: reduction in costs of inspection and rejection. This research addresses the problem of estimating changes moments in time series, in order to reduce the time required to look for assignable causes of variation to help reduce cost of inspection, rejections, and downtime. One approach to address this problem is by obtaining estimators of the change-points that have occurred. This also could answer a question previously proposed by Arunajadai (2009, p.58): "Are the data homogeneous and if not, what are the locations of the homogeneous segments in the data?"

For a single sustained change, most approaches suppose previous knowledge of initial parameters (when in practice in several cases this is not true, for instance, in Phase I of SPC), while, in this research, this assumption is not considered. Change-point estimators when parameters (before and after sustained changes occur) are unknown will be developed by using maximum likelihood methodology due to maximum likelihood estimators (MLEs) provides the more likely values of the true parameters according to all available information. Assumptions made by the proposed solution model are that changes had really occurred and data is normally distributed. A change-point of the series (or process) is defined here as a change in distribution parameters' values and three different cases are

addressed: (1) Change only in mean, (2) change only in variance and (3) change in both parameters at the same time. The results of this approach will be compared with those found in the literature in order to evaluate their performance in terms of accuracy and effectiveness in order to determine which estimator is recommended to use in each situation.

Situations where a process is out of control and multiple change-points have occurred has been worked mostly through applications for shifts in the mean and Bayesian approach as can be found in Fotopoulos, Jandhyala, and Khapalova (2010). In this research MLEs for multiple change-points are developed as well as two heuristics algorithms (evolutionary and constructive) to avoid computational cost due to change-points MLEs time required to obtain them increases in a non-polynomial way which could lead in a retard in searching assignable causes of variation. Similarly to one sustained change, three cases are considered in this problem: (1) k changes only in mean, (2) k changes only in variance and (3) k changes in both parameters at the same time. Finally, simulation will be performed in order to show the behavior of these estimators.

1.3 Research Questions.

This research is two folded: the first one is focused on single step change-point problem, and second one, on multiple step changes. Since previous works in literature usually assume prior knowledge of parameters, it follows that:

Q.1. Does maximum likelihood change-point estimators exist when there is not previous knowledge of parameters for time series normally distributed in which k sustained changes occurred? This is not a trivial question, since MLEs do not always exist.

Questions addressed in each research are presented in its respective subsection.

1.3.1. Research 1: Maximum Likelihood Change-Point Estimators for Normally Distributed Series with Unknown Parameters.

In this research, change-point MLEs were developed for time series normally distributed with a single step change, considering three different cases: (1) change only in mean, (2) change only in variance, (3) change in both parameters at the same time. Change-point estimators found in literature, which are sensitive to: shifts in the mean (CUSUM estimator; Pettitt, (1980)), and shifts in variance (Hawkins and Zamba, (2005a)), were used to compare with. Finally, integration with Quesenberry's Control Charts (Q-charts) (Quesenberry, 1991a, 1991b, 1991c) is presented in order to show its application in on-line monitoring. The sub-questions addressed in this research are:

- \triangleright Q.1.1. What is the bias and spread of estimators in cases (1), (2) and (3)?
- Q.1.2. In which scenarios MLEs' performance is better than CUSUM and Hawkins estimators by means of accuracy and effectiveness?
- Q.1.3. What is the bias and spread of the change-point MLEs after signals of Q-Charts?

1.3.2. Research 2: Maximum Likelihood Estimators for Multiple Change-Points.

In this research, change-points MLEs for time series with multiple changes were developed as well as heuristic (evolutionary algorithm) and constructive algorithms to assess the problem of finding MLEs, which is a non-polynomial (NP) optimization problem. Three cases are considered: (1) k changes only in the mean, (2) k changes only in variance and (3) k changes in both parameters at the same time. Performance of MLEs and heuristics is shown by considering few scenarios. Questions:

- Q.2.1. Is the multiple change-point estimation obtained by the Maximum Likelihood methodology solving time increasing in a non-polynomial way as number of changes increases?
- \triangleright Q.2.2. What is the bias and spread of estimators in cases (1), (2) and (3)?
- Q.2.3. Is the evolutionary algorithm better than constructive algorithm at estimating multiple change-point in terms of time? In terms of bias and spread?

1.4 General Hypothesis.

The general hypothesis of this research is:

H1. It is possible to develop the change-point (single or multiple) maximum likelihood estimators for parameters as well as for change-points when prior knowledge of parameters does not exist.

1.4.1. Research 1: Hypothesis.

The following hypotheses are proposed for research 1:

- H1.1. Bias and spread of change-point MLEs tends to be smaller compared to CUSUM and Hawkins ones when change in both mean and variance occurred at same time. When there is only change in mean or only change in variance, CUSUM and Hawkins estimators biases and spread tends to be smaller than its corresponding change-point MLEs.
- ➢ H1.2. Change-point MLEs' performance is better than CUSUM and Hawkins performance when size of the series is big in means of bias and spread.
- H1.3. Change-point MLE's performance is precise and accurate when it is used after a Q-chart signal.

1.4.2. Research 2: Hypothesis.

The following hypotheses are proposed for research 2:

- ➢ H2.1. The problem of finding multiple change-point MLEs correspond to optimization problem because of solving time increases in a non-polynomial way.
- \blacktriangleright H2.2. What is the bias and spread of estimators for cases (1), (2) and (3)?.
- H2.3. Evolutionary algorithm proposed here is more accurate than constructive algorithm developed here for cases considered here: (1), (2) and (3), but it requires more computational time than constructive.

1.5 Research Purpose.

This research is mainly focused on developing change-point estimators for single and multiple step changes for normally distributed series. These estimators are expected to be as close as possible to the true change-points locations. Even though there are estimators for such data yet, the case when parameters (before and after the change) are unknown has been almost not worked in literature, and that case could be presented in practice. Moreover, by showing that these tools have less bias and spread in several scenarios than others estimators found in literature, particularly, Pettit's CUSUM (1980) for shifts in the mean and Hawkins' (2005a) estimators for shifts in variance.

In other words, development of tools for system management which could help in identification of assignable/special causes of variation which might be eliminated according to third postulate of quality (Shewhart (1931)) is the main purpose. Determine whether or not a process is in control is a task relegated to control charts, as it can be seen with change-point MLE's integration with Q-charts.

1.6 Research Objective.

Let $x_{i,j}$ be random variables following:

$$x_{i,j} \sim \begin{cases} n(\mu_1, \sigma_1^2) \ if \ 1 \le i \le \tau_1; \ 1 \le j \le n \\ n(\mu_2, \sigma_2^2) \ if \ \tau_1 < i \le \tau_2; \ 1 \le j \le n \\ \vdots \\ n(\mu_{m+1}, \sigma_{m+1}^2) \ if \ \tau_m < i \le T; \ 1 \le j \le n \end{cases}$$
(1)

Where τ_k for k = 1,2,...,m are called the series' change-points; j is the number of replications and μ_r, σ_r^2 for r = 1,2,...,m+1 are the parameters of the normal distribution in each sub-section and are unknown as well as the change-points.

Objective 1: Derive the change-points MLEs $\vec{\tau} = \langle \hat{\tau}_1, \hat{\tau}_2, ..., \hat{\tau}_k \rangle$ for change-points of the series $\tau = \langle \tau_1, \tau_2, ..., \tau_k \rangle$ for different cases:

Case 1:
$$\mu_k \neq \mu_{k+1}$$
; $\sigma_1^2 = \sigma_2^2 = ... = \sigma_{m+1}^2 = \sigma_p^2$; $\forall k = 1, 2, ..., m$. (2)

Case 2:
$$\mu_k = \mu_{k+1} = \mu; \ \sigma_k^2 \neq \sigma_{k+1}^2; \ \forall k = 1, 2, ..., m.$$
 (3)

Case 3:
$$\mu_k \neq \mu_{k+1}$$
; $\sigma_k^2 \neq \sigma_{k+1}^2$; $\forall k = 1, 2, ..., m.$ (4)

Objective 2: If k = 1, show that change-point MLE $\hat{\tau}$ for (2), (3) and (4) bias and spread tends to be lower as size of the series increases. Also show that change-point MLE (4) is more precise and accurate than Pettitt's (1980) CUSUM and Hawkins' (2005a) estimators. Objective 3: If k = 1, show change-point MLE $\hat{\tau}$ integration with Q-charts. Objective 4: If k > 1, show that change-point estimation is a NP Problem.

Objective 4. If k > 1, show that change-point estimation is a full resolution

Objective 5: Develop heuristics for multiple change-points MLEs.

Objective 6: Show that heuristics' performance is similar to MLEs (in cases where they could be compared).

1.7 Delimitations.

The next sub-sections present the assumptions and limitations addressed by them.

1.7.1. Assumptions.

The following assumptions were made in the model:

1.- Observations are independent random variables following (1).

2.- It is known a priori that k changes have already occurred over the process.

3.- It is considered that a change have occurred when one or both parameters distribution change.

4.- Parameters before and after each change-point as well as change-points locations are unknown.

5.- Time is considered discrete, not continuous.

1.7.2. Limitations.

Under assumptions made above, the following limitations appear:

With assumption of prior knowledge of that k changes have already occurred, three limitations addressed:

- It is necessary to know the number of changes that have occurred in order to obtain better estimations by using this procedure. Due to control charts only could help to determine if the process is out of control but are not capable to ensure that changes have already occurred.
- When changes have occurred and the control chart signals that, they not provide a clue of the type of change, thus, changes with trend are not covered, such as the case when machines wear out.
- Even when a control chart provides a signal of a process out of control, this signal could be a false alarm, but change-point estimators always determine a point of the time series of where it is more likely that the change have occurred according with the information provided. That is, this procedure could lead to an estimation of change-points, but this "change" could not be considered as statistically significant.

There are some techniques which could help to estimate the number of changes in a time series, like CUSUM control charts of Page (1954). Nevertheless, this research assumes prior knowledge of the number of changes. Finally, hypothesis test is recommended to use to determine if there is a significant change-point in the series, but it is left as future work because it is beyond the research scope. It is noteworthy that normality assumption is not senseless because in practice, the data collection is often with replications, and then limit central theorem ought to be applied.

1.8 Relevance of this study.

The relevance of this study lies in the development of procedures to manage a system and assist in quality control for more cases under the SPC label. Change-points MLEs when parameters (before and after a change have occur) are unknown have not been developed

before. Maximum likelihood procedure was chosen because of its properties: they provided the most likely value of the parameters under estimation, and they are asymptotically unbiased, that is to say, if sample size tends to infinity, then estimator tends to be unbiased.

Multiple change point problem has many applications in natural phenomena and Medicine as can be found in Arunajadai (2009) and Fotopoulos et al. (2010). However, almost all of the cited works there were done from a Bayesian approach, and maximum likelihood procedures were almost not found in literature.

Even though control charts are important because they are useful to determine whether the process is in control, they are not capable to determine the change-points, which could retard the process improvement and leads in a waste of resources. Nonetheless, without that information provided by them no inferences about the change-point could be determined. This suggests that both tools should be used in a complementary way. So, change-point estimators boost the improvement process by giving one location in which start to searching special/assignable causes of variation. That is why integration with these estimators with Q-charts is presented as usefulness and necessary tools.

1.9 Research Outputs and Outcomes.

The major output of this research is the procedure to assist process management when there is not prior knowledge about distributions parameters, that is to say, Phase I of SPC. The following outcomes will be addressed:

1. – Change-points MLEs.

2. – Integration of change point MLE's with Q-charts giving a procedure to system managers.

3. – Multiple change-point estimations by heuristics based on MLE's in order to avoid the computational time problem addressed in this case.

4. – Procedure that helps in decision-making process for system managers.

CHAPTER 2. LITERATURE REVIEW.

2.1. Introduction.

Statistical Process Control (SPC) is used to reduce variation leading to improvement in the performance of processes (Amiri and Allahyari, 2011) .There are two phases in SPC: Phase I in which parameters are estimated with historical data assuming that process is in statistical control whereas in Phase II the process is monitored: new data is tested to being in control according to information provided in the previous phase. Most common tools used in Phase II are control charts which use was explained in previous chapter Phase II is monitoring phase in which it is desirable to determine whether a change have occurred. Amiri and Allahyari (2011) classified different types of changes that have been studied, in which process get out of control: step changes, multiple step changes, changes with drift and monotonic changes which are a mixture of latter ones. In this section, it will be shown the connection of SPC and Change–point analysis going through those techniques and approaches used before CPA was defined and later.

2.2. SPC and Change-Point Analysis.

First tools developed under SPC label were control charts, which are tools that are used to monitor a process and detect assignable and special causes of variation Amiri and Allahyari (2011). Control limits are calculated and then when one or more than one observations fall outside that limits, then it is suspected that a change occurred. In 2007, Koutras, Bersimis, and Maravelakis (2007) classified control charts in 3 major categories: (1) Shewhart's control charts, which have their name after Shewhart (1931); CUSUM control charts, developed by Page (1954); and Exponentially Weighted Moving Average first proposed by Roberts (1959). Shewhart's control charts were created to determine if the process mean and/or variance changed along the time by choosing control limits as the values that are three standard deviations over or above the process mean. Nevertheless, these charts are not sensitive to small shifts and could not detect them while CUSUM and EWMA charts are capable to do that. First ones use a cumulative sum between observations and its average; if there is a sudden change in the slope of the CUSUM, then a change have occurred; second

ones, EWMA's control charts, assign larger weights to new observations in order to avoid no detections of small shifts.

All of these tools are good determining whether or not the process is under statistical control (which is the first step at system management), but when the process is out of control, it is desirable to know at which moment that happened and then apply corrective actions, and control charts have a delay at reporting that in almost all cases. The search of this moment is called change-point problem and change-point analysis was defined by Potts (2003) as a method to find thresholds in relationships between two variables. Taylor (2000) shows differences between use of control charts and CPA (the first one controls point-wise error rate while last ones, the change-wise error rate) and how they can be used in a complementary way in SPC.

2.3. Literature review for Change-Point Analysis (CPA).

Change-point problem was firstly worked, from a Bayesian approach, by Girshick and Rubin in 1952. They proposed quality control rules which have to be applied after a change in a random process was detected. Problem of determine the initial moment of a change has been worked from several approaches: parametric, non-parametric, Bayesian and regression. From parametric approach, almost all works found are about developing MLE's, control charts and tests based on Likelihood Ratio (LR) tests. On the other hand, from a nonparametric approach, transformations of data to another with known distributions were worked. These works are detailed in the next subsections but summarized in Table 1.

Approach	Author(s).	Contributions.
	Page (1954)	CUSUM charts.
metric	Hinkley (1970)	Developed change-point MLE for change in process mean and a statistic. Also derived their asymptotic distributions.
Para	Hinkley (1971)	Derived asymptotic distribution of CUSUM estimator as well as of its statistic.
	Samuel, Pignatiello, and	Change-point MLE using Shewhart's X control
	Calvin (1998a)	chart, for a change in mean.

	Samuel, Pignatiello, and Calvin (1998b)	Change-point MLE for a change in variance using S or R control charts.
	Samuel and Pignatiello (1998)	MLE for Poisson parameter.
	Timmer, Pignatiello, & Longnecker, (1998)	Control chart for changes in AR(1) time series.
	Jann (2000)	Change-point estimator for multiple changes in normal processes with shifts in the mean using a genetic algorithm.
	Dabye and Kutoyants (2001)	MLE for Poisson using boundaries.
	Samuel and Pignatiello (2001)	MLE for binomial's p parameter.
	Nedumaran, Pignatiello and Calvin (2002)	MLE for changes in mean of Normal Multivariate processes.
	Timmer and Pignatiello (2003)	MLE for changes in AR(1) processes.
	Hawkins and Zamba (2005a)	Control chart based on GLR test using Bartlett's test for changes in variance. Parameters unknown.
	Zamba and Hawkins (2006)	Control chart based on LR test for change in mean of multivariate normal processes.
	Liming (2008)	MLE for autoregressive time series.
	Reynolds and Jianying (2010)	Control chart based on GLR for shifts in the mean of normal processes.
	Fotopoulos (2010)	Derived the exact asymptotic distribution of change-point MLE in a computable form.
	Cordero et al. (2012)	Control chart based on χ^2 test for changes in variance.
	Tercero et al. (2012)	Control chart for change in variance based on F test.
	Chen and Gupta (2012)	Compiled Parametric CPA works.
	Tercero et al. (2013a)	Integration of change-point MLE with a self- starting CUSUM for normally distributed series.
tric	Page (1955)	Use the sign function to determine changes in the known initial mean parameter for symmetric distributions.
arame	Bhattacharyya and Johnson, (1968)	Test for shift in the mean of observations which has a symmetric cumulative distribution.
Von-P	Pettitt (1979)	Nonparametric test for Bernoulli, Binomial or continuous distributions.
4	Pettitt (1980)	CUSUM based statistic for Bernoulli observations.

Hinkley, D. V., and Schechtman, E. (1987)	Bootstrap method for shifts in the mean process.
Ghazanfari, et al. (2008)	Clustering technique to estimate change-points for normal or non-normal distributed time series with shifts in the mean.
Ghazanfari, M.,	Clustering method capable to estimate change-
Alaeddini, A., and	points and parameters values after a change in
Noghondarian, K. (2008)	the mean.
Harchaoui, Bach, and Moulines (2009)	Test statistic for homogeneity of two-subsamples and derived its asymptotic null distribution
Tercero, G., Temblador, M., Beruvides, M. and Hernández A. (2013b)	Change-point estimator using p-value of Mood's median Test for random walks with drift.

Table 1. Summary of CPA literature review.

2.3.1. Parametric Approach CPA.

Page (1954) started this line of research with his CUSUM control charts. Even though this procedure dos not estimate the initial moment of a change, gives a signal that a change have already occurred (Tercero (2011)). MLEs were considered by first time for Hinkley (1970). He developed MLEs for changes for independent random variables normally distributed for Phase II of SPC as well as LR tests. After that, Hinkley (1971) derived the asymptotic distribution of the MLE for changes in the mean when parameters are known or unknown, but it was not presented in a computable form. This could be considered as the base work. Next works are presented in three different categories: Estimation, Control Charts, and Ratio Tests.

Change-point MLEs following Hinkley's (1971) guideline were developed by the following authors. (Samuel, Pignatiello, and Calvin, 1998a) developed change-point MLE for a change in the mean of normally distributed data which is used after a signal of a Shewhart's \overline{X} chart assuming in-control mean as known. In the same year, Samuel, Pignatiello and Calvin (1998b), developed the change-point MLE for change in variance of normally distributed observations and used it after a signal of a dispersion control chart such as S or R charts assuming initial parameters known. They also evaluate its

performance over different subgroup sizes and changes in variance measured in ratio of deviations.

Change-points MLEs for other distributions were also developed. Samuel and Pignatiello (1998) proposed an estimator for a step change in a Poisson rate parameter, using the same analysis of their previous works. Dabye and Kutoyants (2001) also worked with this distribution but they demonstrate consistency of the change-point MLE by considering boundaries. MLE for Binomial distribution p parameter was developed by Pignatiello and Samuel (2001) and its performance was evaluated after a signal given by a p or np chart along different values of p. For multivariate normal process with a change in mean, Nedumaran, Pignatiello and Calvin (2000) developed the change-point MLE and evaluated its performance over different scenarios. Liming (2008) proposed some statistic for change-point problem for autoregressive time series models with both cases of variance known or unknown.

Control charts integration with change-point estimators were first done by Timmer, Pignatiello, and Longnecker (1998), they proposed a test for monitoring the level parameter of AR(1) processes which resulted in a CUSUM-based control chart. Later, Timmer and Pignatiello (2003) proposed three estimators for the parameters of such that model, using their previous control charts. Reynolds and Jianying (2010) developed a control chart using a moving window based on GLR methodology for small shifts in the mean of normally distributed data. Using GLR, Cordero et al. (2012) and Tercero et al. (2012) developed control charts and change-point estimators for changes in variance in normally distributed data using the *F* test and the χ^2 test for Phases I and II, respectively. In 2013, Tercero et al. (2013a) integrated the change-point MLE for shifts in the mean after a signal of a selfstarting CUSUM.

Hypothesis tests were worked by several authors after Hinkley's (1970) work. Hawkins and Zamba (2005a) developed a LR test based on Bartlett's test for mean and variance of normally distributed data using only one test for all cases: change only in mean, only in

variance or both parameters. After that, Zamba and Hawkins (2006) developed a LR Test for multivariate normal processes with shifts in the mean. Fotopoulos et al. (2010) continued Hinkley's (1970) work and derived the exact asymptotic distribution of the MLE for changes in the mean as well as the LR Statistic obtaining good approximations of the actual MLE distribution.

Several parametric CPA works were compiled by Chen and Gupta (2012) in 2012, including estimation, LR tests, and change-point null distribution. This monograph also includes applications of CPA for single and multiple change-point problems.

2.3.2. Nonparametric Approach CPA.

Assessing the problem from a nonparametric perspective, Page (1955) proposed a method to identify changes in the process mean where initial parameter was known using the sign function: $y_i = \text{sgn}(x_i - \theta)$ for symmetric distributions. Later, Bhattacharyya and Johnson (1968) worked in this approach, testing a shift in the process mean when initial parameter are known and unknown, only by assuming symmetry of observation's cumulative distribution. Pettitt (1979) worked with binomial, Bernoulli and continuous observations obtaining approximate and exact results about testing null hypothesis of no change, stated as $\tau = T$ where τ is the change-point location and T is the size of the sample data. Later, Pettitt (1980) developed a simple cumulative sum type test and a conditional test of no change comparing this with the likelihood test. The estimator developed by him was also compared with the MLE for one-zero observations showing that his estimator performs generally superior to MLE. Bootstrap technique were used by Hinkley and Schechtman (1987) to develop estimators for models with a shift in the mean and compared its performance with parametric and semi-parametric methods. Jann (2000), construct a cost function to determine the number of changes in normal distributed processes with shifts only in the mean using a genetic algorithm based on the t-test. Later, Ghazanfari, et al. (2008) get away from normal series and developed a technique based on clusters to estimate change-points obtaining that true values of the in-control and out of control parameters of the process are estimated effectively. In the same year, Ghazanfari,

Alaeddini, and Noghondarian (2008) devised a new clustering method capable to estimate the time at which a sustained shift in the mean occurred as well as for true values of the out of control process' parameters. Based on the maximum kernel Fisher discriminant ratio Harchaoui, Bach, and Moulines (2009) proposed a test statistic which was developed as an indicator of homogeneity of two sub-samples, and, when this statistic indicates that a change have occurred also gives an estimation of the change-point. They derive the asymptotic distribution of their statistic under null hypothesis of no change as well as its consistency under alternative hypothesis of change. Recently, Tercero et al. (2013b) developed a change-point estimator for random walks with drift using the p-value of the Mood's median test.

2.3.3 General Remarks.

There are several approaches to solve the change-point problem as well as types of changes: single step changes, multiple step changes, changes with linear trend, and monotonic changes according to Amiri and Allahyari's (2011) literature review. This research considers only parametric approach for single and multiple step changes in time series. Under this label, many approaches of solution suppose initial parameters as known; other works have approximate or asymptotic results for the estimator's distributions.

Change-point problem could be addressed from other approaches, like Bayesian and Regression in which there are the following works: Girshick and Rubin (1952), first proposed the Change-point problem from a Bayesian point of view. For stationary observations, several approaches were proposed by Shiryaev (1963), Chernoff and Zacks (1964), Barry and Hartigan (1993), Chib (1998), and Moreno, Casella and García-Ferrer (2005). For non-stationary observations, Ferreira (1975) studied trended observations with normal errors, developing estimator and confidence intervals for change-point. Multiple linear regression models were studied by Holbert (1982) and Chen (1998). Finally, Western and Kleykamp (2004) developed a change-point estimator for the coefficients of a regression line using simulation methods.

About multiple change points, according to Jann (2000) and Fotopoulos et al. (2010) there are several researches focused mainly in application of CPA like meteorology, analysis of DNA sequences, signal processing, econometrics, and statistical process control. A vast number of researches were found for climate data analysis trying to find change-point in rainfalls records (or find inhomogeneities in climatological time series): Potter (1981), Maronna and Yohai (1978), Easterling and Peterson (1995), Lanzante (1996), Alexandersson and Moberg (1997). For DNA sequences, Arunajadai (2009) presents a methodology to model the RNA unwinding mechanism using Tukey's biweight function to detect changes in the mean. Fu and Curnow (1990) studied Bernoulli independent variables sequences, and derived the MLE distribution of the location of two changed segments to predict protein helical regions. Finally, tests for multiple change-point have been developed by Huskova and Slaby (2001), and Aly, Abd-Rabou and Al-Kandari (2003).

For a literature review, see Amiri and Allahyari (2011), and Chen and Gupta (2012). Amiri and Allahyari (2011) summarized works categorized by approach of solution, change-point estimation method, parameter consider for the change, and control chart used (if is the case). Chen and Gupta (2012), compiled in a book several focused in the parametric approach and works for applications to genetics, medicine and finance.

CHAPTER 3. RESEARCH 1.

Change-Point Estimation for a Sequence of Normal Observations and Integration with Q-Charts

This is the first research of change-point analysis for independent observations normally distributed. It considers the case when a single step change has occurred and distribution's parameters (before and after change) are unknown. Development of maximum likelihood estimators (MLEs) for the change-point and for parameters is the main concern as well as an integration with control charts in order to show its application in practice, with which retrospective and on-line analysis are both covered. A change is considered as one of the three different cases: (1) change only in mean parameter, (2) change only in variance parameter or (3) change in both parameters. Due to there are change-point estimators for change in mean and change in variance, a comparison is done to show what estimator is recommended to use in each situation.

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Change-Point Estimation for a Sequence of Normal Observations and Integration with Q-Charts.

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Many practical applications have to deal with situations where parameters are unknown and have to be estimated from collected data where a structural change happened at an unknown change-point. This situation is found during start-up processes, root cause analysis performed over past observations, and many other situations where backward-looking examination for a change-point in some measured variable is required. This paper presents and evaluates the performance of three maximum likelihood estimators (MLE) of the change-point in series for retrospective analysis and online monitoring through the sequential use with Q-charts. Process parameters, before and after a change, are assumed to be unknown. Different shifts, sample sizes, and locations of change-points were evaluated. For retrospective analysis, a comparison is made with estimators based on cumulative sums and Bartlett's test. Performance analysis done with extensive simulations showed that the MLEs perform better (or equal) in almost every scenario, with smaller bias and standard error. Integration with Q-charts showed that the sequential use of both methodologies facilitates the detection and estimation of special causes of variations, fostering any quality improvement effort. Strategies to reduce bias and standard error of estimators through the use of additional observations are also presented.

Keywords: MLE; CUSUM; Bartlett's Test; unknown parameters; change-point analysis

3.1. Introduction

Control charts are known tools to detect isolated and sustained changes. However, when sustained changes occur, most of them are not capable of estimating the initial moment of the change. Knowing this exact time greatly simplifies the search for a cause of variation, and in consequence, might boost an improvement process. The search for this moment is called change-point estimation. Potts (2003) defines it as methods created to identify thresholds in the relationship between two variables; however, it can be generalized for multiple changes. From a parametric point of view, following the guidelines of Hinkley (1970), several authors like Samuel et al. (1998a) and Khoo (2004) have studied the behaviour of the maximum likelihood estimators (MLE) for a change-point of a normal process. These authors studied the behaviour of these estimators where a priori knowledge of initial parameters existed. Nevertheless, real life applications usually lack this information, and parameters have to be estimated from collected data.

This research is focused on the construction and performance evaluation of several changepoint MLEs for normal observations collected over a discrete time where parameters before and after the change-point are unknown. Given a time series of independent observations $X_{1,1},...,X_{1,n},...,X_{\tau,1},...,X_{\tau,n}, X_{\tau+1,1},...,X_{\tau+1,n},...,X_{T,1},...,X_{T,n}$ following the subsequent model:

$$X_{i,j} \sim \begin{cases} N(\mu_0, \sigma_0), & 1 \le i \le \tau, 1 \le j \le n \\ N(\mu_1, \sigma_1), & \tau < i \le T, 1 \le j \le n \end{cases}$$
(1)

Where parameters τ , μ_0 , μ_1 , σ_0 and σ_1 are unknown. τ is called the change-point of the series, and T is the last sample observed. To estimate the change-point, three MLE estimators called $\hat{\tau}_{MLE1}$, $\hat{\tau}_{MLE2}$, and $\hat{\tau}_{MLE3}$ are obtained based on three different scenarios, according to different assumptions about parameters of the normal distribution.

 $\hat{\tau}_{MLE1}$ assumes that $\mu_0 \neq \mu_1$ but $\sigma_0 = \sigma_1$. $\hat{\tau}_{MLE2}$ assumes that $\sigma_0 \neq \sigma_1$ but $\mu_0 = \mu_1$. $\hat{\tau}_{MLE3}$ assumes that $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$. To measure the performance of these estimators, this research evaluated, with extensive simulations, different scenarios where the size of the shift, sample size, and the change-point position were modified to measure the sensitivity of estimators. Results are compared with estimators from Pettitt (1980) and Hawkins and Zamba (2005a). Additionally, to extend the applicability of the proposed estimators, integration with Q-charts is proposed and their performance is evaluated.

Section 3.2 presents an overview of the research in change-point analysis, and briefly describes Q-charts with their related literature. The research showed no indication of the existence of an in-depth study of the biases and errors of the proposed estimators when applied in retrospective analysis for limited sample sizes. Neither was any study found about their performance when used sequentially with Q-charts. Section 3.3 presents the proposed change-point estimators. Section 3.4 shows how change-point estimators can be integrated with Q-charts. Experimental results from Monte Carlo simulations are described in Section 3.5; and finally, some general conclusions and opportunities for future research are mentioned in Section 3.6.

3.2. Background

3.2.1 Previous Work on Change-Point Analysis

Concerns of detecting sustained changes in time series started with Girshick and Rubin (1952) from a Bayesian paradigm. They defined a quality control rule to trigger corrective actions when a change in a random process was detected. Soon after, Page (1954, 1955, 1957), from a frequentist point of view, developed the cumulative sum (CUSUM) chart to be able to detect, faster than traditional Shewhart's control charts (1931), the presence of sustained changes.

Hinkley (1970) sets the theoretical foundation to construct MLEs and likelihood ratio (LR) tests to detect change points in series of independent random variables. He applied these techniques to series with normally distributed observations. Following this theory, Samuel, Pignatiello, and Calvin (1998a, 1998b), Samuel and Pignatiello (1998), Dabye and Kutoyants (2001), Pignatiello and Samuel (2001), Nedumaran, Pignatiello, and Calvin

(2002), Timmer and Pignatiello (2003) and Liming (2008) developed MLEs for series following different distributions. They focused their work on the integration with control charts, where the MLEs were used as a plug in to estimate the change already detected. To detect if a change had happened, Timmer, Pignatiello, and Longnecker (1998) worked on a LR test based on the CUSUM chart to detect changes in a first order autoregressive process. Hawkins and Zamba (2005b), and Zamba and Hawkins (2006) and Batsidis (2010) worked on several LR tests to make inferences whether a change has occurred in individual stationary series. Hawkins and Zamba (2005a) presented a model to deal with variance changes, similar to the generalized likelihood ratio (GLR) control chart for variance, based on Bartlett's test. Nevertheless, the proposed model grew in complexity as more observations were added into the time series. To solve the complexity issue of the GLR when dealing with mean changes, Reynolds and Jianying (2010) simplified the approach by suggesting the application of a moving window, where the amount of steps required with each new observation was restricted to the size of the window.

Aside from MLE procedures, Ghazanfari et al. (2008) proposed the use of clustering principles to identify two partitions, within the time line, where the probability of an observation of belonging to one of the two sets in the series was used as a separation criterion. Page (1954), when developing the CUSUM, first pointed that results from this technique could be used to estimate the initial time of the change. Hinkley (1971) compared the later estimation with the MLE for known initial parameters of normal and independent observations, concluding that the use of the CUSUM is asymptotically biased, but easier to use. Pettitt (1980) proposed the estimation with CUSUM for unknown parameters, and Nishina (1992) evaluated the performance against estimations obtained from EWMA and Moving Average charts, determining that estimation from CUSUM was superior, and, if the size of the change is known a priori, he proved that the estimation with the CUSUM was an MLE.

For nonstationary series, Quandt (1958) first constructed a MLE and LR test for observations following two different schemes in a regression line with normally distributed errors. Later, several LR tests were built by Kim and Siegmund (1989), Zou, Zhang, and

Wang (2006), Perry, Pignatiello, and Simpson (2006), Mahmoud, Parker, Woodall, and Hawkins (2007) and Zhou, Zou, Zhang, and Wang (2009). All of these tests assumed normally distributed errors and were designed to detect changes in the intercept and the slope of trended series.

On the other hand, Bayesian statisticians continued with the research line initiated by Girshick and Rubin (1952). For stationary observations, several approaches were proposed by Shiryaev (1963), Chernoff and Zacks (1964), Barry and Hartigan (1993), Chib (1998) and Moreno, Casella, and Garcia-Ferrer (2005). For non-stationary observations, Ferreira (1975) developed an estimator and confidence intervals for the change-point of trended observations with normal errors. Holbert (1982) and Chen (1998) also worked with change-point analysis for multiple linear regression models. Finally, Western and Kleykamp (2004) designed a change-point estimator for the coefficients of a regression line using simulation methods.

Bhattacharyya and Johnson (1968) were responsible for the first construction of a nonparametric test with the explicit idea of doing a nonparametric method. However, Page (1955) was the first one to develop a nonparametric change-point detection technique. He applied the CUSUM technique to the dichotomy created by the sign of the difference between observations in a time series and a specification. Later, Pettitt (1979) used nonparametric techniques to change-point analysis by developing tests for Bernoulli, binomial and continuous observations. A year after, Pettitt (1980) approached the CUSUM for zero-one observations, similar to the one built by Page (1955). Finally, Hinkley and Schechtman (1987) applied the re-sampling technique, the bootstrap, to estimate the moment of a shift in the mean. Tercero et al. (2013b), also from a nonparametric perspective, using the p-value of Mood's median test (1954), constructed an estimator capable of detecting changes in the median of time series. Recently, Zou et al. (2007) proposed the use of the empirical likelihood ratio to approach the change-point test and estimation problems.

To assess situations where the assumption of independent observations is not met, Perry and Pignatiello (2010) developed a MLE for a step change in the mean of stationary and invertible ARMA processes. Latter, Perry (2010) derived and evaluated the MLE for the time of polynomial change in mean of covariance-stationary autocorrelated process. Finally, Perry and Pignatiello (2012) obtained a MLE for the change point in the fixed-effects components in a two stage-nested random model.

For series of normally and independently distributed observation, many MLEs for known parameters have been developed and studied. However, when dealing with real life situations, parameters are usually unknown. Even when parameters are assumed to be known, most of the time they were estimated from historical data. From the reviewed literature, change-point estimation for unknown parameters hasn't been deeply studied, and its construction and performance needed to be addressed. The following section introduces the MLEs for unknown parameters under three different circumstances when mean and variance are assumed to be equal or different. Pettitt (1980) and Hawkins and Zamba (2005a) estimators are also presented.

3.2.2 Q-Charts for Normal Observations

Quesenberry (1991a, 1991b, 1991c) developed several control charts, called Q-charts, capable of monitoring sequences of observations under different scenarios of a priori knowledge about the population parameters of a process when it follows a Normal distribution, Binomial or Poisson. Shewhart type control charts follow an implementation paradigm of two phases. Phase I, also called estimation phase, is focused on finding a set of in-control observations that can be used to estimate the parameters of the in-control state of the process under consideration. Control limits that represent the variation under common causes are set at this stage. During Phase II, the system is monitored, and all parameters estimated in previous phase are considered as the population parameters. To avoid biases and underperformance during a Phase II, large amount of data need to be obtained when parameters are estimated. This might be unreasonable when samples are limited and the process needs to be monitored from early stages. By considering the estimation error, Quesenberry modified several Shewhart charts that can be used for start-up processes with short and long runs. Four of these Q-charts are considered in this research since they make

no assumptions about none of the true values of parameters in normal sequences of independent observations. These are the control charts for mean and variance for individual observations and rational subgroups where samples have at least two observations each. Charts formulas are shown in equations (2-11).

Q control chart for individual observations. Here r stands for the moment in time.

$$\bar{x}_r = \frac{\sum_{i=1}^r x_i}{r}$$
(2)

$$s_r^2 = \frac{\sum_{i=1}^r (x_i - \bar{x}_r)^2}{r - 1}$$
(3)

$$Q_r(x_r) = \Phi^{-1} \left\{ G_{r-2} \left[\left(\frac{r-1}{r} \right)^{\frac{1}{2}} \left(\frac{x_r - \overline{x}_{r-1}}{s_{r-1}} \right) \right] \right\}, \ r = 3, 4, \dots$$
(4)

Where G_{r-2} and Φ^{-1} are for the t distribution with r – 2 degrees of freedom and the inverse normal standard distribution.

Q control chart for mean using rational subgroups.

$$\overline{\overline{x}}_{r} = \frac{\sum_{i=1}^{r} n_{i} \overline{x}_{i}}{n_{1} + \dots + n_{r}}$$

$$\tag{5}$$

$$s_{p,r}^{2} = \frac{\sum_{i=1}^{r} (n_{i} - 1)s_{i}^{2}}{n_{1} + \dots + n_{r} - r}$$
(6)

$$W_{r} = \sqrt{\frac{n_{r}(n_{1} + n_{2} + \dots + n_{r-1})}{n_{1} + n_{2} + \dots + n_{r}}} \left(\frac{\overline{x}_{r} - \overline{\overline{x}}_{r-1}}{s_{p,r}}\right), \ r = 2,3,4,\dots$$
(7)

$$Q_r(\bar{x}_r) = \Phi^{-1} \{ G_{n_1 + n_2 + \dots + n_{r-1}}(W_r) \}, \ r = 2, 3, 4, \dots$$
(8)

Q control chart for process variances with individual observations

$$R_r = x_r - x_{r-1} (9)$$
$$Q_r(R_r) = \Phi^{-1} \left\{ F_{1,\nu} \left(\frac{\nu R_r^2}{R_2^2 + R_4^2 + \dots + R_{r-2}^2} \right) \right\}, \ r = 4, 6, \dots; \ \nu = \frac{r}{2} - 1$$
(10)

Q control chart for process variances using rational subgroups.

$$W_r = \frac{(n_1 + \dots + n_{r-1} - r + 1)s_r^2}{(n_1 - 1)s_1^2 + \dots + (n_{r-1} - 1)s_{r-1}^2}$$
(11)

$$Q_r(s_r^2) = \Phi^{-1} \{ F_{n_r - 1, n_1 + n_2 + \dots + n_{r-1} - r+1}(W_r) \}, \ \mathbf{r} = 2, 3, 4, \dots$$
(12)

Q-charts belong to the area of self-starting control charts. This type of control charts deal with the problem of monitoring processes without the need of a previous estimation of process parameters. This problem was first assessed by Hawkins (1987) by adapting the CUSUM chart to include running estimators of mean and variance. Later Quesenberry (1991a, 1991b, 1991c) used this approach to create self-starting Shewhart-type control charts (as previously presented) for Normal, Binomial, and Poisson observations. Zou et al. (2007) applied linear regression results to develop a self-starting control chart to monitor several related variables called linear profiles. He et al. (2008) proposed a different running estimator of the variance to reduce the bias of Q-charts when a change happened early (a bias occurs when the out-of-control ARL is larger than in-control ARL when a change does exist). To improve power of self-starting charts, Capizzi and Masarotto (2012) used EWMA statistics over Quesenberry's Q variables, and applied a CUSCORE control chart for monitoring. Sullivan and Jones (2002) extended previous works to construct a self-starting Multivariate EWMA control chart. A similar job was done by Hawkins and Maboudou-Tchao (2007).

3.3. Change-Point Estimators

Following the theory developed by Hinkley (1970), three different scenarios are studied, giving three different estimates: mean changes (Section 3.3.1), variance changes (Section 3.3.2), and mean and variance change at the same time (Section 3.3.3). Derivation of these MLEs is shown below. Pettitt (1980) and Hawkins and Zamba (2005a) estimators are reviewed in Sections 3.3.4 and 3.3.5 respectively.

Let { $x_{ij}: i = 1, 2, ..., \tau, j = 1, 2, ..., n$ } be independent and identically distributed random variables (i.i.d.r.v.) $N(\mu_0, \sigma_0)$, and{ $x_{ij}: i = \tau + 1, \tau + 2, ..., T, j = 1, 2, ..., n$ } be i.i.d.r.v. $N(\mu_1, \sigma_1)$. For a given value of τ , the likelihood function is

$$L(\mu_{0},\mu_{1},\sigma_{0},\sigma_{1}|\vec{x}) = \prod_{i=1}^{\tau} \prod_{j=1}^{n} f(x_{ij}|\mu_{0},\sigma_{0}) \cdot \prod_{i=\tau+1}^{T} \prod_{j=1}^{n} f(x_{ij}|\mu_{1},\sigma_{1})$$
(13)

Then

$$\log L = -nT \log(\sqrt{2\pi}) - n \log(\sigma_0) - n(T - \tau) \log(\sigma_1) - \frac{1}{2\sigma_0^2} \sum_{i=1}^{\tau} \sum_{j=1}^{n} (x_{ij} - \mu_0)^2 - \frac{1}{2\sigma_1^2} \sum_{i=\tau+1}^{T} \sum_{j=1}^{n} (x_{ij} - \mu_1)^2$$
(14)

MLEs are found by solving equations (15-17) for $\mu_0, \mu_1, \sigma_0, \sigma_1$ and τ . Results are shown in the following three sections.

$$\frac{\partial \log L}{\partial \mu_0} = \frac{\partial \log L}{\partial \mu_1} = \frac{\partial \log L}{\partial \sigma_p^2} = 0$$
(15)

$$\frac{\partial \log L}{\partial \mu} = \frac{\partial \log L}{\partial \sigma_0^2} = \frac{\partial \log L}{\partial \sigma_1^2} = 0$$
(16)

$$\frac{\partial \log L}{\partial \mu_0} = \frac{\partial \log L}{\partial \mu_1} = \frac{\partial \log L}{\partial \sigma_0^2} = \frac{\partial \log L}{\partial \sigma_1^2} = 0$$
(17)

3.3.1 MLE with $\mu_0 \neq \mu_1$ and $\sigma_0 = \sigma_1$

This scenario assumes that, between τ and $\tau + 1$, a change occurs only in the mean $(\mu_0 \neq \mu_1)$, but not in the standard deviation $(\sigma_0 = \sigma_1)$. Since all parameters are unknown, they are all estimated using the MLE technique. Equations (18-20) show the corresponding MLEs for the parameters of a normal distribution. Equation (21) gives the change-point MLE of the model shown in equation (1) with corresponding assumptions of this scenario.

$$\hat{\mu}_{0} = \frac{\sum_{i=1}^{\tau} \sum_{j=1}^{n} x_{ij}}{tn}$$
(18)

$$\hat{\mu}_{1} = \frac{\sum_{i=\tau+1}^{T} \sum_{j=1}^{n} x_{ij}}{(T-t)n}$$
(19)

$$\hat{\sigma}_{p}^{2}(\hat{\mu}_{0},\hat{\mu}_{1}) = \frac{\sum_{i=1}^{\tau} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{0})^{2} + \sum_{i=\tau+1}^{T} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{1})^{2}}{n\mathrm{T}}$$
(20)

$$\hat{\tau}_{MLE1} = \underset{5 \le \tau \le T-5}{\operatorname{arg\,min}} \left\{ \hat{\sigma}_{p} \left(\hat{\mu}_{0}, \hat{\mu}_{1} \right) \right\}$$
(21)

Note that change-point MLEs omit the first and last five samples of the series. This is done to avoid the undesirably tendency of these MLEs to favour the locations of change-point at the beginning or end of the series, as suggested by Karl Tr. and Williams CN Jr. (1987). This was also suggested in Jann (2000) who estimates multiple change-points in normal series using an iterative method based on the t-statistic. This assumption of not having a change-point within the first and last five samples is used when constructing the other estimators in this section.

3.3.2 MLE with $\mu_0 = \mu_1$ and $\sigma_0 \neq \sigma_1$

This scenario assumes that after moment τ a change occurs only in the standard deviation $(\sigma_0 \neq \sigma_1)$, but not in the mean $(\mu_0 = \mu_1)$. Using the MLE technique all unknown parameters are estimated. Equations (22) and (23) show the corresponding MLEs for the variances (before and after the change). The estimator of μ , $\hat{\mu}_p$, is obtained after solving equation (24), which is actually a third degree polynomial equation with at least one real solution out of three possible ones, which need to be evaluated individually using equation (25). The latter equation gives the MLE change-point of the model from equation (1) with the conditions of this second scenario.

$$\hat{\sigma}_{0}^{2}(\hat{\mu}_{p}) = \frac{\sum_{i=1}^{\tau} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{p})^{2}}{n\tau}$$
(22)

$$\hat{\sigma}_{1}^{2}(\hat{\mu}_{p}) = \frac{\sum_{i=\tau+1}^{T} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{p})^{2}}{n(T-\tau)}$$
(23)

$$\frac{1}{\hat{\sigma}_{0}^{2}(\mu)}\sum_{i=1}^{\tau}\sum_{j=1}^{n}(x_{ij}-\mu)+\frac{1}{\hat{\sigma}_{1}^{2}(\mu)}\sum_{i=\tau+1}^{T}\sum_{j=1}^{n}(x_{ij}-\mu)=0$$
(24)

$$\hat{\tau}_{MLE2} = \underset{5 \le \tau \le T-5}{\operatorname{argmin}} \left\{ \hat{\sigma}_0^t \left(\hat{\mu}_p \right) \hat{\sigma}_1^{T-\tau} \left(\hat{\mu}_p \right) \right\}$$
(25)

It can be shown that the Hessian Matrix of σ_0^2 and σ_1^2 is defined negative, independently of the value of μ (see proof in Tercero-Gómez (2011) when n = 1). Nevertheless, equation (24) has three different roots (including imaginary ones), and an evaluation of the loglikelihood function is required to choose the maximum out of the real results. Equation (26) shows the corresponding loglikelihood function without the constant values. Given any t, it can be seen, on equation (26), that as $\mu \rightarrow \infty$ or $\mu \rightarrow -\infty$ then $\ln L < 0$, hence, the MLE for μ exists, and it can be found by evaluating the roots obtained in equation (24) on equation (26).

$$\log L = -n\tau \log(\hat{\sigma}_{0}(\hat{\mu}_{p})) - n(T-\tau)\log(\hat{\sigma}_{1}(\hat{\mu}_{p})) - \frac{1}{2\hat{\sigma}_{0}^{2}(\hat{\mu}_{p})} \sum_{i=1}^{\tau} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{p})^{2} - \frac{1}{2\hat{\sigma}_{1}^{2}(\hat{\mu}_{p})} \sum_{i=\tau+1}^{T} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{p})^{2}$$
(26)

3.3.3 MLE with $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$

This third scenario assumes that after moment τ a change occurs in both parameters $(\mu_0 \neq \mu_1)$ and $(\sigma_0 \neq \sigma_1)$. Since all parameters are unknown, all of them are estimated using the MLE technique. Equations (18) and (19) show the corresponding MLEs for the means. Equations (22) and (23) are used to calculate the variances $\hat{\sigma}_0^2(\hat{\mu}_0)$ and $\hat{\sigma}_1^2(\hat{\mu}_1)$, where $\hat{\mu}_0$ and $\hat{\mu}_1$ are used instead of $\hat{\mu}_p$. Equation (27) gives the MLE change-point of the model from equation (1) with the conditions of this third scenario.

$$\hat{\tau}_{MLE3} = \underset{5 \le \tau \le T-5}{\operatorname{argmin}} \left\{ \hat{\sigma}_0^{\tau} \left(\hat{\mu}_0 \right) \hat{\sigma}_1^{T-\tau} \left(\hat{\mu}_1 \right) \right\}$$
(27)

If variance values are smaller than 1, the minimization process over equations (21, 25 and 27) can be made over the logarithms of these functions to reduce the risk of rounding errors.

3.3.4 Change-Point estimation with CUSUM for shifts in mean

From Pettitt (1980), estimation of the change-point for mean shifts is obtained by finding the maximum absolute deviation from the overall mean. Deviation is calculated according to equation (28) and the change-point estimator is given in (29).

$$U_{t} = \sum_{i=1}^{t} \left(X_{i} - T^{-1} \sum_{i=1}^{T} X_{i} \right)$$
(28)

$$\hat{\tau}_{CUSUM} = \inf_{t_0} \left\{ t_0 : \left| U_{t_0} \right| \ge \left| U_t \right|; t = 1, \dots, T \right\}$$
(29)

If subgroups exist, mean values within each subgroup of X_i observations are used as if they were individual observations.

3.3.5 Change-Point estimation with Bartlett's test statistic

To assess for variance changes, Hawkins and Zamba (2005a) used the Bartlett's test statistic and the GLR approach to create a change-point estimator. The change-point estimator is obtained by finding the moment t where equation (30), Bartlett's test statistic, is maximized. This equation uses equations (18) to (20), (22) and (23) to obtain values for $\hat{\mu}_0$, $\hat{\mu}_1$, $\hat{\sigma}_0^2(\hat{\mu}_0)$, $\hat{\sigma}_1^2(\hat{\mu}_1)$ and $\hat{\sigma}_p^2(\hat{\mu}_0, \hat{\mu}_1)$.

$$G_{t} = \frac{(nt-1)\log\left[k_{1}\frac{\hat{\sigma}_{p}^{2}(\bar{\mu}_{0},\bar{\mu}_{1})}{\hat{\sigma}_{0}^{2}(\bar{\mu}_{0})}\right] + (n(T-t)-1)\log\left[k_{2}\frac{\hat{\sigma}_{p}^{2}(\bar{\mu}_{0},\bar{\mu}_{1})}{\hat{\sigma}_{1}^{2}(\bar{\mu}_{1})}\right]}{C}$$
(30)

Where:

$$C = 1 + \left[(nt-1)^{-1} + (n(T-t)-1)^{-1} - (nT-2)^{-1} \right] / 3$$
(31)

$$k_1 = \frac{T(nt-1)}{t(nT-2)}$$
(32)

$$k_2 = \frac{T(n(T-t)-1)}{(T-t)(nT-2)}$$
(33)

In consequence, Hawkins and Zamba's (2005a) change-point estimator can be written as

$$\hat{\tau}_G = \underset{2 \le t \le T-2}{\operatorname{arg\,max}} \{ G_t \}$$
(34)

3.4. Sequential Use of Change-Point Estimators and Control Charts

In the presence of sustained changes, Q-charts and $\hat{\tau}_{MLE}$ can be used sequentially for online monitoring. Control charts can be used to detect whether a change occurred, and the MLE's can be applied to estimate the initial moment of the sustained change. Process monitoring is done using Q-charts until a sample gives an out-of-control signal. This last sample is defined as T from model (1). Then, a change-point MLE is used to estimate the initial moment of the change.

To monitor mean changes, Q-charts for individual observations and mean values are used with $\hat{\tau}_{MLE1}$. To assess for changes in scale, Q-chart for variance with individual observations or subgroups are used together with $\hat{\tau}_{MLE2}$. If changes in both parameters at the same time are a concern, Q-charts for mean and variance can be used at the same time by adjusting their corresponding control limits to obtain a desired ARL under control. $\hat{\tau}_{MLE3}$ can be used after a change is detected using the previous control scheme.

3.5. Performance of Estimators

3.5.1 Retrospective Analysis: Simulation Design

To evaluate performance of $\hat{\tau}_{MLE1}$, $\hat{\tau}_{MLE2}$, $\hat{\tau}_{MLE3}$, $\hat{\tau}_{CUSUM}$ and $\hat{\tau}_{G}$, several scenarios were simulated by considering the following factors and levels:

- 1. Shift in the mean (δ) was measured in standard deviations from an initial mean. Shifts considered were σ , 1.5 σ and 3 σ .
- 2. Ratio of deviations (σ_1/σ_0) measures the amount of change in a process standard deviation. Ratios of 1.3, 1.5 and 3 were considered.
- 3. Series length (*T*) of 50, 100, 300 and 1000 samples were simulated. Each sample having different sizes, depending on the scenario studied.
- 4. Subgroup sizes (*n*) of 1, 3 and 5 were evaluated.
- 5. Change-point position (τ/T) of 0.2, 0.3 and 0.5 were used to measure how standard error of estimators improves as subgroups get larger.

Monte Carlo experimentation was used to evaluate the performance of the change-point estimators. The following general procedure was used for each scenario evaluated:

- 1. Select the scenario from a combination of the factors and levels shown above.
- 2. Generate nT random variables according to the selected scenario.
- 3. Calculate $\tau \hat{\tau}$ (using estimators under analysis).
- 4. Repeat step 2 and 3 10,000 times.
- 5. Calculate the mean and standard deviation of the error (the latter is also called standard error).
- 6. Return to step 1 and select another scenario.

3.5.2 Online Monitoring with Q-Charts: Simulation Design

To evaluate the performance of the sequential application of estimators $\hat{\tau}_{mle1}$, $\hat{\tau}_{mle2}$ and $\hat{\tau}_{mle3}$ with Q-charts, several scenarios were assessed using Monte Carlo simulation. A sensitivity analysis was completed in order to evaluate bias and standard deviation of the online monitoring. Factors and their corresponding levels studied are similar to the ones evaluated for retrospective analysis, shift in the mean (δ) was also measured in standard deviations σ , 1.5 σ and 3 σ . Ratios of standard deviations (σ_1/σ_0) of 1.3, 1.5 and 3 were studied. Subgroup size, or sample size (n) also considered values of 1, 3 and 5. The difference in performance assessments between retrospective analysis and online monitoring is in the change-point position. The ratio τ/T no longer can be used. Series

length is no longer a fixed value but a random variable. Change-point position is now set for specific τ moments 50 and 100. Simulations were run setting up Q-charts to provide an in-control ARL of 370.4. To evaluate performance of $\hat{\tau}_{mle3}$, Q-charts for mean and variance were used at the same time. The latter scheme had control limits of ±3.205 on each chart to provide the same in-control ARL of a 3-sigma chart, 370.4.

Once in a while Q-charts misbehave, giving large ARL values if the change is not detected within certain time window. This creates excessive computational times that make some computers run out of memory. To avoid this, the maximum series length allowed was 500 per replicate. If no out-of-control signal was triggered after 500 samples, the replicate was run again. This reduces performance of change-point estimators since the amount of data to estimate the change is reduced. However, as seen in the simulation results, bias and standard error still behaves relatively well enough to make conclusions about the feasibility and performance of integrating Q-charts with change-point estimators.

The procedure applied to evaluate integration between Q-charts and MLEs for each scenario is described below:

- 1. Select the scenario using a combination of factors and levels as described above.
- 2. Generate $n\tau$ observations in control according to the selected scenario and make $i = \tau$.
- 3. Generate another observation out of control under the scenario selected and make i = i + 1. If $i \ge 500$ repeat from step 2.
- 4. If *i* triggers and out-of-control signal with the Q-chart, then make T = i and go to step 5. If not, repeat step 3.
- 5. Calculate $\tau \hat{\tau}$ (using estimators under analysis).
- 6. Repeat step 2 to 4 10,000 times.
- 7. Calculate the mean and standard deviation of the error.
- 8. Return to step 1 and select another scenario.

3.5.3 Simulation Results

When $\mu_0 \neq \mu_1$ and $\sigma_0 = \sigma_1$, $\hat{\tau}_{MLE1}$ and $\hat{\tau}_{CUSUM}$ were evaluated over different series length (T), sample sizes (n), shifts of the mean (δ) measured in standard deviations, and changepoint locations (τ/T). Table 2 part a) shows, when $\tau/T = 0.5$, that $\hat{\tau}_{MLE1}$ and $\hat{\tau}_{CUSUM}$ perform with similar biases—with a difference between estimators of at most ± 0.1 —but $\hat{\tau}_{CUSUM}$ presents a smaller standard error than $\hat{\tau}_{MLE1}$. However, when $\tau/T \neq 0.5$ (Table 2 part b)), $\hat{\tau}_{MLE1}$ tends to always have a smaller bias and standard error. Considering that, in practice, an analyst is not assumed to know beforehand when the change actually occurred, then $\hat{\tau}_{MLE1}$ is the recommended estimator, because it is more robust to the change-point location.

Performance results of $\hat{\tau}_{MLE2}$ and $\hat{\tau}_G$ when $\mu_0 = \mu_1$ and $\sigma_0 \neq \sigma_1$ are shown in Table 3. There can be seen, when $\tau/T = 0.5$, $\hat{\tau}_{MLE2}$ and $\hat{\tau}_G$ have almost the same performance. Biases and standard errors are within ± 1 in most cases (in both parts a) and b)). $\hat{\tau}_G$ tends to have a bigger bias but a smaller standard error, mostly for smaller samples. However, when samples are large enough $\hat{\tau}_{MLE2}$ and $\hat{\tau}_G$ performs alike. On the other hand $\hat{\tau}_G$ requires less operations to be obtained, hence less computer time.

If it is not possible to assume that only one parameter changed at the change-point, one should assume $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$. Tables 4 and 5 compare this situation using $\hat{\tau}_{MLE3}$ with $\hat{\tau}_{CUSUM}$ and $\hat{\tau}_G$. In Table 4, using a $\tau/T = 0.5$, when comparing part (a) versus part (b), it can be seen that as the ratio of standard deviations increases, the error bias and standard error of the $\hat{\tau}_{CUSUM}$ also increase, while the $\hat{\tau}_{MLE3}$ improves its precision. Table 4 (c) shows that $\hat{\tau}_G$ performs relatively well when there is no change in the mean, only in variance, its bias is similar to the $\hat{\tau}_{MLE3}$ and the standard error is smaller. Nevertheless, when $\delta > 0$, bias and standard error of $\hat{\tau}_{MLE3}$ tend to be smaller than $\hat{\tau}_G$ in every case. Table 5 confirms the superiority of $\hat{\tau}_{MLE3}$ over $\hat{\tau}_{CUSUM}$ and $\hat{\tau}_G$ when changes in mean and variance occur at different τ/T . In almost every case, $\hat{\tau}_{MLE3}$ give a smaller bias and standard error.

Additionally, when comparing $\hat{\tau}_{MLE3}$ with $\hat{\tau}_{MLE1}$ and $\hat{\tau}_{MLE2}$ it can be seen that performance of $\hat{\tau}_{MLE3}$ is not bad (absolute bias is smaller than the unit in most cases and standard error is similar). This makes $\hat{\tau}_{MLE3}$ a safe choice when compared with the other estimators that need to assume that only one parameter changed.

Following the model presented in Section 3.4, for online monitoring, when $\mu_0 \neq \mu_1$ and $\sigma_0 = \sigma_1$, $\hat{\tau}_{MLE1}$ performance was evaluated after integrating it with Q-charts. Table 6 shows that in almost every situation, $\hat{\tau}_{MLE1}$ bias and standard error get smaller when Q-charts' ARL become larger, and that behavior is reversed when the ARL gets smaller, $\hat{\tau}_{MLE1}$ bias and standard error tend to get bigger. This can be expected since small ARL means quick detection and not many observations after the real change-point. If this happens, change-point is located close to the end of the series. Because the search of the change-point is limited to be at least 5 observations before the end of the series, the feasible region of search might not contain the real change-point. This leaves change-point estimator with not much data to work with, making bias and standard error bigger. This situation can be solved by letting the process run 5 extra observations after the change is detected.

Also, for online monitoring, performance of $\hat{\tau}_{MLE2}$ after its integration with Q-charts when $\mu_0 = \mu_1$ and $\sigma_0 \neq \sigma_1$ was evaluated and results are shown in Table 6. Results of integration of Q-charts with $\hat{\tau}_{MLE2}$ shows that for almost every case, bias and standard error are greatly corrected by adding at least 5 observations of the out of control process after Q-charts' detection.

Finally, when $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$, performance of $\hat{\tau}_{MLE3}$ was evaluated in Table 7. These tables show that for smaller samples bias and standard error is larger. This gets corrected by adding replications and/or new extra observations after Q-charts integration. In Tables 6 and 7, *w* extra observations were added to estimate the change-point. Maximum likelihood estimators improve their performance when more observations are used. However, this growth in precision implies an increase in the cost of the out of control observations

produced. An analyst should consider if the increment in precision overcomes the cost of having additional observations after a change is signaled by a Q-chart.

3.6. Conclusions and Future Work

This paper presented three estimators of the change-point in series of independent normal observations that deal with changes in the mean, the variance, and in both parameters at the same time. Estimators were obtained by maximizing the likelihood function of time series when there is an unknown change at moment τ and the mean and variance before and after the change are also unknown. Some of these estimators can be found in past literature; however there was no indication about their performance with fixed samples and their relationship with variance minimization (it was shown that all estimators could be written as a variance minimization problem). Also, no reference was found about estimator $\hat{\tau}_{MLE2}$, probably due to the lack of a single solution for the mean estimator that needed to be used. However, it was shown that $\hat{\tau}_{MLE2}$ was in fact a MLE since it provides a global maximum for the likelihood function.

The MLEs here proposed were evaluated over different shifts, sample sizes, and locations of change-points; and they were compared with two estimators, one based on the cumulative sum (CUSUM) and the other on Bartlett's test. The former, the CUSUM estimator, was designed to detect the moment when a change occurred in the mean of normal observations, and the latter, when the change happened in the variance. Performance was measured using extensive simulations, showing that the MLEs perform better (or equal) in almost every scenario when compared with their counterparts. Bias and standard error was generally smaller with the MLEs. Nonetheless, it is important to notice that CUSUM based estimators are easier to compute, and their performances could be acceptable in some situations, making them an alternative when only rough estimates are needed. These estimators can be used for retrospective analysis or as part of online control with unknown parameters control charts as presented here. The performance of MLEs when used after a signal of Q control charts was inspected. Sequential use of this control

charts and MLEs improves the bias of the change-point estimator. It was found that large changes create small ARL values. This means that not many observations might be available to estimate the change-point, which is reflected as an increase in bias and standard error. If precision is a must, to solve this situation, the use of at least 5 additional observations after a change is detected is recommended.

Future work will deal with other types of situations seen in a Phase I or II of SPC. It is known that types of changes found in a sequence of Phase I process data are not necessarily that of a single shift. Instead, if the system is out-of-control, multiple change points might be at hand in the form of shifts in mean, variance, drifts of a trend, seasonality, outliers, or a combination of these over independent or autocorrelated observations. Future research will focus on the development of multiple change-points, autocorrelated data, and nonnormal observations through nonparametric change-point estimators.

3.7. References

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3.8. Appendix.

Table 2. Performance of change-point estimators when $\mu_0 \neq \mu_1$ and $\sigma_0 = \sigma_1$.

Change-point estimations using $\hat{\tau}_{MLE1}$ and $\hat{\tau}_{CUSUM}$ are evaluated over different series length (T), sample sizes (n), shifts of the mean (δ) measured in standard deviations and change-point locations (τ/T). Estimations are presented next to their corresponding standard error, which are within parentheses.

				· · ·			
		$\hat{ au}_{MLE1}$			$\hat{ au}_{ ext{cusum}}$		
Т	n	$\delta = 1$	$\delta = 1.5$	$\delta = 3$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
	1	-0.04 (5.69)	0.03 (2.84)	0.00 (0.53)	-0.04 (3.61)	0.03 (1.93)	-0.01 (0.46)
50	3	-0.02 (2.02)	0.00 (0.77)	0.00 (0.11)	-0.03 (1.49)	0.00 (0.66)	0.00 (0.10)
50	5	-0.02 (1.05)	0.00 (0.43)	0.00 (0.03)	-0.02 (0.85)	0.00 (0.36)	0.00 (0.03)
	1	0.01 (6.44)	-0.03 (2.64)	0.00 (0.53)	0.02 (4.12)	-0.01 (2.06)	0.00 (0.50)
100	3	0.01 (1.82)	0.02 (0.75)	0.00 (0.10)	0.00 (1.51)	0.01 (0.69)	0.00 (0.10)
	5	0.00 (1.02)	-0.01 (0.42)	0.00 (0.03)	0.01 (0.94)	-0.01 (0.38)	0.00 (0.03)
	1	0.03 (5.56)	-0.01 (2.30)	0.00 (0.49)	0.03 (4.57)	-0.01 (2.17)	0.00 (0.48)
300	3	0.00 (1.73)	0.00 (0.71)	0.00 (0.09)	0.00 (1.62)	0.01 (0.69)	0.00 (0.09)
	5	-0.01 (0.98)	0.00 (0.38)	0.00 (0.03)	0.00 (0.94)	0.00 (0.37)	0.00 (0.03)
1000	1	0.09 (5.20)	0.01 (2.28)	-0.01 (0.50)	0.07 (4.93)	0.00 (2.23)	0.00 (0.50)
	3	-0.01 (1.63)	0.00 (0.70)	0.00 (0.10)	-0.01 (1.61)	0.01 (0.69)	0.00 (0.10)
	5	0.00 (1.00)	0.00 (0.38)	0.00 (0.03)	0.00 (0.98)	0.00 (0.38)	0.00 (0.03)

Part a) $\tau/T = 0.5$.

Part b) $\delta = 1.5$

			$\hat{ au}_{_{MLE1}}$			$\hat{ au}_{ ext{CUSUM}}$	
Т	п	$\tau/T = 0.2$	$\tau/T = 0.3$	$\tau/\mathrm{T}=0.5$	$\tau/T = 0.2$	$\tau/T = 0.3$	$\tau/\mathrm{T}=0.5$
	1	0.73 (3.82)	0.26 (3.04)	0.02 (2.73)	3.26 (4.86)	1.47 (2.99)	0.03 (1.85)
50	3	0.38 (1.07)	0.01 (0.81)	0.00 (0.79)	1.81 (2.24)	0.53 (1.21)	0.00 (0.66)
	5	0.02 (0.44)	0.00 (0.42)	-0.01 (0.39)	0.82 (1.59)	0.31 (0.80)	-0.01 (0.35)
	1	0.24 (3.22)	0.12 (2.70)	-0.01 (2.51)	3.96 (6.34)	1.72 (3.55)	-0.02 (2.01)
100	3	0.33 (0.93)	0.02 (0.74)	-0.01 (0.74)	1.96 (2.64)	0.57 (1.34)	-0.01 (0.67)
	5	0.00 (0.42)	0.00 (0.38)	0.00 (0.39)	0.83 (1.69)	0.30 (0.79)	0.01 (0.38)
	1	0.05 (2.40)	0.01 (2.37)	-0.03 (2.35)	4.47 (7.81)	1.86 (4.09)	-0.02 (2.14)
300	3	0.31 (0.86)	0.00 (0.72)	-0.01 (0.71)	2.14 (3.09)	0.60 (1.43)	-0.01 (0.70)
	5	0.01 (0.39)	0.00 (0.38)	0.00 (0.40)	0.87 (1.84)	0.32 (0.83)	0.00 (0.39)
	1	0.03 (2.27)	-0.01 (2.33)	0.01 (2.25)	5.06 (9.33)	1.92 (4.26)	0.01 (2.17)
1000	3	0.30 (0.90)	-0.01 (0.70)	-0.01 (0.68)	2.24 (3.33)	0.60 (1.42)	-0.01 (0.68)
	5	0.00 (0.39)	0.00 (0.38)	0.00 (0.41)	0.90 (1.88)	0.32 (0.86)	0.00 (0.40)

Table 3. Performance of change-point estimators when $\mu_0 = \mu_1$ and $\sigma_0 \neq \sigma_1$

Change-point estimations using $\hat{\tau}_{MLE2}$ and $\hat{\tau}_{G}$ are evaluated over different series length (T), sample sizes (*n*), shifts in the ratio of deviations (σ_1/σ_0) and change-point locations (τ/T). Estimations are presented next to their corresponding standard error, which are within parentheses.

Part a) $\tau/T = 0.5$.

			$\hat{ au}_{\scriptscriptstyle MLE2}$			$\hat{ au}_{_G}$	
Т	Ν	$\sigma_1/\sigma_0 = 1.3$	$\sigma_1/\sigma_0=1.5$	$\sigma_1/\sigma_0 = 3$	$\sigma_1/\sigma_0 = 1.3$	$\sigma_1/\sigma_0 = 1.5$	$\sigma_1/\sigma_0 = 3$
	1	-1.15 (12.20)	-1.10 (10.15)	-0.76 (3.00)	-0.88 (14.36)	-0.88 (11.88)	-0.78 (2.92)
50	3	-0.60 (9.24)	-0.63 (5.99)	-0.16 (0.81)	-0.65 (10.69)	-0.65 (6.54)	-0.16 (0.80)
	5	-0.74 (7.18)	-0.45 (3.93)	-0.06 (0.43)	-0.63 (8.07)	-0.44 (4.08)	-0.06 (0.43)
	1	-1.67 (24.25)	-1.48 (17.40)	-0.80 (2.73)	-1.27 (26.82)	-1.18 (18.45)	-0.81 (2.71)
100	3	-0.87 (14.51)	-0.91 (6.86)	-0.14 (0.75)	-1.05 (15.47)	-0.93 (6.96)	-0.15 (0.76)
	5	-0.68 (9.52)	-0.51 (3.87)	-0.05 (0.41)	-0.71 (9.82)	-0.50 (3.86)	-0.05 (0.41)
	1	-2.43 (48.80)	-3.21 (21.57)	-0.79 (2.39)	2.52 (50.44)	.3.20 (21.24)	-0.80 (2.40)
300	3	-1.81 (16.24)	-0.85 (5.84)	-0.15 (0.72)	-1.81 (16.04)	-0.86 (5.84)	-0.15 (0.72)
	5	-0.95 (8.79)	-0.49 (3.46)	-0.05 (0.42)	-0.94 (8.84)	-0.49 (3.45)	-0.05 (0.42)
	1	-4.90 (47.74)	-3.26 (17.08)	-0.78 (2.35)	-4.96 (47.25)	-3.26 (17.23)	-0.78 (2.35)
1000	3	-1.58 (13.71)	-0.92 (5.39)	-0.16 (0.74)	-1.57 (13.73)	-0.92 (5.39)	-0.16 (0.74)
	5	-0.88 (7.81)	-0.47 (3.14)	-0.06 (0.42)	-0.88 (7.80)	-0.47 (3.13)	-0.06 (0.42)

Part b) $\sigma_1/\sigma_0 = 1.5$

			$\hat{ au}_{\scriptscriptstyle MLE2}$			$\hat{ au}_{G}$	
Т	п	$\tau/T = 0.2$	$\tau/T = 0.3$	$\tau/T = 0.5$	$\tau/T = 0.2$	$\tau/T = 0.3$	$\tau/T = 0.5$
	1	-9.74 (12.66)	-6.15 (11.11)	-1.01 (10.16)	-10.24 (14.51)	-6.36 (12.87)	-0.73 (11.82)
50	3	-4.15 (8.54)	-2.10 (6.78)	-0.59 (5.92)	-4.54 (9.88)	-2.23 (7.61)	-0.60 (6.51)
	5	-1.83 (5.76)	-0.97 (4.37)	-0.37 (3.84)	-1.87 (6.40)	-1.06 (4.78)	-0.40 (4.00)
	1	-11.88 (23.32)	-7.08 (19.50)	-1.40 (17.43)	-12.78 (25.36)	-7.44 (21.20)	-1.34 (18.59)
100	3	-3.08 (10.48)	-1.57 (7.97)	-0.88 (6.71)	-3.27 (11.16)	-1.64 (8.14)	-0.92 (6.81)
	5	-1.06 (5.35)	-0.67 (4.11)	-0.43 (3.79)	-1.11 (5.54)	-0.67 (4.09)	-0.43 (3.79)
	1	-8.77 (34.84)	-4.90 (24.65)	-2.66 (21.09)	-9.19 (35.57)	-5.27 (25.45)	-2.68 (21.04)
300	3	-1.57 (6.89)	-1.05 (6.04)	-0.95 (5.89)	-1.63 (6.90)	-1.05 (6.00)	-0.94 (5.90)
	5	-0.53 (3.40)	-0.54 (3.56)	-0.48 (3.24)	-0.54 (3.43)	-0.55 (3.57)	-0.48 (3.24)
1000	1	-3.83 (20.22)	-3.38 (18.02)	-2.92 (17.12)	-4.04 (20.35)	-3.48 (17.96)	-2.94 (16.96)
	3	-1.40 (5.57)	-0.94 (5.40)	-0.91 (5.30)	-1.41 (5.61)	-0.96 (5.44)	-0.91 (5.30)
	5	-1.40 (5.57)	-0.94 (5.40)	-0.91 (5.30)	-0.47 (3.24)	-0.46 (3.25)	-0.48 (3.24)

Table 4. Performance of change-point estimators when $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$

Given a T = 100 and τ/T = 0.5, change-point estimations using $\hat{\tau}_{MLE3}$ are evaluated in part (a), $\hat{\tau}_{CUSUM}$ in part (b), and $\hat{\tau}_{G}$ in part (c) over different ratios (σ_{1}/σ_{0}), sample sizes (*n*), and shifts in the mean (δ). Mean values are next to their corresponding standard error within parentheses.

$\sigma_{_1}/\sigma_{_0}$	n	$\delta = 0.0$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
	1		-0.04 (8.11)	-0.03 (2.62)	0.00 (0.53)
1.0	3	N/A	0.01 (1.83)	0.01 (0.75)	0.00 (0.10)
	5		0.03 (1.06)	0.00 (0.40)	0.00 (0.02)
	1	-1.82 (20.27)	-0.99 (8.02)	-0.62 (3.74)	-0.09 (0.82)
1.5	3	-0.89 (7.49)	-0.28 (1.97)	-0.12 (0.97)	-0.01 (0.19)
	5	-0.41 (4.07)	-0.14 (1.10)	-0.05 (0.55)	0.00 (0.08)
	1	-0.77 (2.73)	-0.73 (2.41)	-0.65 (2.22)	-0.38 (1.24)
3.0	3	-0.15 (0.78)	-0.13 (0.69)	-0.11 (0.60)	-0.05 (0.34)
	5	-0.05 (0.41)	-0.04(0.37)	-0.04 (0.32)	-0.01 (0.15)

Part (a). Performance of the MLE $\hat{\tau}_{\rm \scriptscriptstyle MLE3}$

Part (b). Performance of the CUSUM estimator $\hat{\tau}$	CUSUM •
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$\sigma_{_1}/\sigma_{_0}$	п	$\delta = 0.0$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
	1	N/A	-0.03 (4.28)	-0.01 (1.95)	0.00 (0.49)
1.0	3	1N/A	0.02 (1.48)	0.01 (0.70)	0.00 (0.09)
	5		0.02 (0.96)	0.00 (0.37)	0.00 (0.02)
	1	-10.54 (19.48)	-1.91 (6.06)	-0.91 (3.17)	-0.21 (0.82)
1.5	3	-10.21 (19.52)	-0.73 (2.53)	-0.31 (1.17)	-0.04 (0.25)
	5	-10.22 (19.75)	-0.43 (1.53)	-0.18 (0.70)	-0.01 (0.12)
	1	-18.39 (13.97)	-8.20 (10.85)	-4.58 (7.34)	-1.42 (2.67)
3.0	3	-18.32 (13.77)	-3.78 (6.28)	-1.90 (3.43)	-0.46 (1.06)
	5	-18.13 (13.77)	-2.43 (4.26)	-1.18 (2.29)	-0.24 (0.64)

Part (c). Performance of the Hawkins' estimator $\hat{\tau}_{_G}$.

$\sigma_{_1}/\sigma_{_0}$	n	$\delta = 0.0$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
	1		0.60 (33.92)	0.35 (30.84)	0.16 (22.29)
1.0	3	N/A	0.21 (31.38)	0.36 (27.36)	-0.26 (20.81)
	5		0.28 (30.28)	0.16 (26.17)	-0.05 (20.37)
	1	-1.26 (18.64)	4.04 (18.06)	8.80 (16.44)	14.45 (10.6)
1.5	3	-0.85 (6.85)	3.60 (7.17)	8.00 (7.64)	14.62 (4.82)
	5	-0.43 (3.91)	2.84 (4.91)	6.88 (5.98)	14.50 (4.00)
	1	-0.77 (2.68)	-0.56 (2.52)	-0.20 (2.53)	1.36 (3.28)
3.0	3	-0.15 (0.77)	-0.07 (0.73)	0.01 (0.72)	0.66 (1.45)
	5	-0.05 (0.42)	-0.02 (0.39)	0.02 (0.41)	0.40 (0.93)

Table 5. Performance of change-point estimators when $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$

Given a fixed $\sigma_1/\sigma_0 = 1.5$, and a shift in mean of $\delta = 1.5$, performance of $\hat{\tau}_{MLE3}$ is evaluated in part (a) and $\hat{\tau}_{CUSUM}$ in part (b), and $\hat{\tau}_G$ in part (c) over different series length (T), sample sizes (*n*), and change-point locations (τ/T). Estimations are presented next to their corresponding standard error, which are within parentheses.

Т	п	$\tau/T = 0.2$	$\tau/\mathrm{T}=0.3$	$\tau/\mathrm{T}=0.5$
	1	-2.38 (7.06)	-1.23 (5.22)	-0.57 (4.16)
50	3	-0.47 (1.57)	-0.18 (1.24)	-0.14 (1.10)
	5	-0.07 (0.63)	-0.06 (0.61)	-0.05 (0.58)
	1	-1.19 (6.53)	-0.79 (4.23)	-0.60 (3.60)
100	3	-0.38 (1.19)	-0.15 (1.09)	-0.12 (1.00)
	5	-0.06 (0.56)	-0.06 (0.58)	-0.04 (0.53)
	1	-0.65 (3.02)	-0.65 (3.01)	-0.58 (3.00)
1000	3	-0.35 (1.07)	-0.13 (0.94)	-0.12 (0.93)
	5	-0.05 (0.52)	-0.04 (0.53)	-0.05 (0.52)

Part (a). Performance of the MLE $\hat{\tau}_{MLE3}$.

Part (b). Performance of the CUSUM estimator $\hat{\tau}_{\rm CUSUM}$.

Т	п	$ au/\mathrm{T}=0.2$	$\tau/T = 0.3$	$\tau/T = 0.5$
	1	-5.61 (6.97)	-3.03 (4.64)	-0.79 (2.69)
50	3	-2.99 (3.81)	-1.24 (2.22)	-0.29 (1.08)
	5	-1.69 (2.77)	-0.76 (1.50)	-0.16 (0.66)
	1	-7.17 (9.92)	-3.73 (5.98)	-0.89 (3.11)
100	3	-3.54 (4.81)	-1.43 (2.62)	-0.31 (1.19)
	5	-1.97 (3.42)	-0.86 (1.73)	-0.18 (0.72)
	1	-11.27 (19.42)	-4.79 (8.68)	-1.15 (3.81)
1000	3	-4.30 (7.01)	-1.60 (3.17)	-0.35 (1.24)
	5	-2.25 (4.27)	-0.89 (1.86)	-0.19 (0.73)

Part (c). Performance of the Hawkins' estimator $\hat{\tau}_{G}$.

Т	п	$\tau/T = 0.2$	$\tau/T = 0.3$	$\tau/\mathrm{T}=0.5$
	1	-9.04 (15.02)	-3.95 (13.26)	3.09 (11.11)
50	3	-2.25 (10.00)	1.04 (6.84)	4.49 (5.56)
	5	0.01 (6.01)	1.62 (3.82)	4.09 (4.06)
	1	-9.88 (27.16)	-0.78 (20.87)	8.78 (16.67)
100	3	0.52 (10.15)	3.36 (6.70)	7.82 (7.62)
	5	1.37 (4.27)	2.75 (4.14)	6.97 (5.86)
	1	9.82 (19.07)	19.08 (26.60)	61.68 (46.20)
1000	3	4.16 (7.97)	10.69 (14.85)	55.11 (32.71)
	5	2.90 (5.42)	7.87 (11.05)	53.52 (27.53)

Table 6. Performance of change-point estimators for on-line analysis for changes in mean and changes in variance, respectively.

Given a fixed change-point located at $\tau = 100$. Performance of $\hat{\tau}_{MLE1}$ and $\hat{\tau}_{MLE2}$ used sequentially with Q-charts for mean and variance were evaluated. Estimations are presented next to their corresponding standard error, which are within parentheses, over different sample sizes (*n*), shifts of the mean (δ) and different ratios of deviations (σ_1/σ_0). ARL of Q-charts is indicated with bold numbers.

		Change in mean			Cł	Change in variance		
п	w	$\delta = 1$	$\delta = 1.5$	$\delta = 3$	σ_1/σ_0 = 1.3	σ_1/σ_0 = 1.5	σ_1/σ_0 = 3	
	ARL	91.11 (108.36)	40.75 (77.97)	2.42 (3.34)	132.52 (112.07)	97.15 (101.73)	9.42 (14.28)	
	0			-18.69				
1		-3.32 (15.53)	-6.36 (18.88)	(28.11)	22.99 (71.27)	4.65 (30.10)	-2.27 (9.73)	
1	5	-0.51 (9.20)	-0.19 (4.32)	-0.02 (0.60)	20.57 (67.52)	5.16 (29.55)	0.50 (4.07)	
	10	-0.20 (7.91)	-0.03 (3.03)	-0.02 (0.52)	17.98 (66.44)	4.90 (28.35)	0.64 (3.24)	
	15	-0.01 (6.68)	0.04 (2.54)	-0.01 (0.52)	16.94 (63.98)	4.61 (27.24)	0.69 (2.66)	
	20	-0.02 (6.55)	-0.01 (2.57)	0.00 (0.51)	15.63 (64.09)	4.26 (25.93)	0.75 (2.68)	
	ARL	10.75 (10.82)	3.10 (2.66)	1.02 (0.13)	81.19 (91.47)	37.33 (57.82)	2.17 (1.69)	
	0		-15.72	-21.03			-6.58	
	0	-6.55 (18.61)	(26.70)	(27.91)	-0.28 (22.89)	-3.06 (15.48)	(14.01)	
3	5	-0.16 (3.10)	-0.04 (0.86)	0.00 (0.11)	1.44 (21.37)	0.10 (10.38)	0.11 (1.05)	
	10	-0.06 (2.13)	-0.02 (0.74)	0.00 (0.09)	1.87 (21.01)	0.62 (7.83)	0.13 (0.78)	
	15	-0.04 (2.02)	-0.01 (0.77)	0.00 (0.11)	1.75 (19.57)	0.72 (7.56)	0.12 (0.74)	
	20	-0.03 (1.92)	0.00 (0.75)	0.00 (0.09)	1.59 (19.05)	0.87 (7.17)	0.15 (0.75)	
	ARL	4.75 (4.33)	1.60 (0.99)	1.00 (0.00)	59.33 (77.74)	17.91 (32.34)	1.37 (0.72)	
	0	-11.76	-23.23	-13.33			-7.68	
	0	(23.90)	(30.36)	(21.39)	-1.92 (16.69)	-4.77 (16.34)	(14.31)	
5	5	-0.07 (1.39)	-0.02 (0.45)	0.00 (0.03)	0.23 (13.34)	-0.05 (6.68)	0.04 (0.43)	
	10	-0.05 (1.10)	-0.02 (0.39)	0.00 (0.01)	0.37 (12.35)	0.25 (4.31)	0.04 (0.40)	
	15	-0.03 (1.03)	-0.01 (0.39)	0.00 (0.01)	0.62 (11.28)	0.31 (4.25)	0.05 (0.39)	
	20	0.00 (1.04)	0.00 (0.41)	0.00 (0.02)	0.90 (10.87)	0.41 (3.73)	0.05 (0.40)	

Table 7. Performance of change-point estimators when $\mu_0 \neq \mu_1$ and $\sigma_0 \neq \sigma_1$, for on-line monitoring.

Given a fixed change-point located at $\tau = 100$. Performance of $\hat{\tau}_{MLE3}$ is evaluated when used with Q-charts. Estimations are presented next to their corresponding standard error within parentheses, over different sample sizes (*n*), shifts of the mean (δ) and different ratios of deviations (σ_1/σ_0). ARL of Q-charts is indicated with bold numbers.

$\sigma_{_1}/\sigma_{_0}$	w	$\delta = 0$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
1	ARL	N/A	95.86 (107.75)	56.09 (92.57)	3.28 (15.12)
	0		-3.68 (16.62)	-5.58 (17.93)	-14.50 (25.33)
	5		-1.17 (11.62)	-0.51 (6.18)	-0.03 (0.98)
	10		-0.62 (9.34)	-0.10 (3.61)	-0.01 (0.60)
	15		-0.41 (8.42)	-0.08 (2.96)	0.00 (0.54)
	20		-0.04 (7.80)	-0.03 (2.76)	0.00 (0.53)
1.5	ARL	31.99 (46.52)	17.96 (33.18)	9.95 (20.66)	2.24 (3.40)
	0	-6.72 (34.51)	-8.66 (23.71)	-9.25 (22.32)	-12.71 (23.24)
	5	-1.71 (31.96)	-1.20 (14.82)	-0.70 (9.31)	0.04 (1.53)
	10	-0.74 (31.05)	-0.23 (11.96)	0.14 (6.06)	0.09 (0.94)
	15	-0.76 (29.34)	0.44 (9.45)	0.44 (4.15)	0.10 (0.88)
	20	-0.01 (27.68)	0.70 (8.40)	0.48 (3.94)	0.09 (0.83)
3	ARL	3.22 (2.83)	2.96 (2.51)	2.73 (2.28)	1.95 (1.40)
	0	-11.77 (23.27)	-11.50 (22.58)	-11.75 (23.01)	-10.69 (20.78)
	5	-0.15 (7.73)	-0.16 (7.21)	0.03 (6.07)	0.28 (2.08)
	10	0.51 (3.99)	0.47 (3.61)	0.50 (2.92)	0.35 (1.20)
	15	0.69 (3.10)	0.60 (2.67)	0.65 (2.13)	0.39 (1.30)
	20	0.71(2.72)	0.73(2.21)	0.62 (1.95)	0.39(1.17)

Part (a) $\tau = 100$ and n = 1.

$\sigma_{_1}/\sigma_{_0}$	W	$\delta = 0$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
1	ARL	N/A	10.36 (10.37)	3.04 (2.60)	1.02 (0.13)
	0		-7.74 (20.65)	-15.42 (26.67)	-12.44 (20.87)
	5		-0.29 (4.03)	-0.07 (1.37)	0.00 (0.12)
	10		-0.09 (2.39)	-0.02 (0.79)	0.00 (0.11)
	15		-0.07 (2.04)	-0.02 (0.76)	0.00 (0.09)
	20		-0.03 (1.93)	-0.01 (0.74)	0.00 (0.11)
1.5	ARL	15.94 (25.42)	4.55 (4.48)	2.45 (1.99)	1.08 (0.29)
	0	-9.39 (24.55)	-11.84 (23.97)	-14.18 (24.91)	-11.47 (20.21)
	5	-1.70 (14.50)	-0.19 (4.78)	0.00 (1.66)	0.00 (0.23)
	10	-0.78 (12.29)	0.13 (2.72)	0.07 (1.08)	0.01 (0.20)
	15	0.17 (9.27)	0.19 (2.08)	0.10 (0.99)	0.01 (0.20)
	20	0.27 (8.65)	0.25 (1.87)	0.11 (0.96)	0.01 (0.21)
3	ARL	1.58 (0.99)	1.49 (0.87)	1.39 (0.76)	1.14 (0.41)
	0	-11.69 (21.34)	-10.60 (19.46)	-10.34 (19.21)	-7.92 (14.94)
	5	0.09 (0.96)	0.09 (0.69)	0.07 (0.62)	0.04 (0.35)
	10	0.14 (0.77)	0.12 (0.66)	0.10 (0.58)	0.05 (0.34)
	15	0.14 (0.75)	0.12 (0.64)	0.11 (0.59)	0.04 (0.32)
	20	0.15 (0.73)	0.13 (0.66)	0.12 (0.60)	0.05 (0.33)

Part (b) $\tau = 100$ and n = 3.

Part (c) $\tau = 100$ and n = 5.

$\sigma_{_1}/\sigma_{_0}$	w	$\delta = 0$	$\delta = 1$	$\delta = 1.5$	$\delta = 3$
1	ARL	N/A	4.66 (4.22)	1.59 (0.97)	1.00 (0.01)
	0		-13.00 (25.03)	-21.89 (29.70)	-6.45 (10.10)
	5		-0.11 (1.88)	-0.03 (0.48)	0.00 (0.02)
	10		-0.02 (1.31)	-0.01 (0.43)	0.00 (0.02)
	15		0.01 (1.19)	-0.01 (0.40)	0.00 (0.03)
	20		0.02 (1.17)	-0.01 (0.42)	0.00 (0.01)
1.5	ARL	10.13 (14.79)	2.83 (2.40)	1.61 (1.01)	1.01 (0.08)
	0	-9.30 (22.49)	-13.19 (22.96)	-15.22 (24.71)	-6.92 (12.01)
	5	-0.73 (9.04)	0.05 (0.81)	0.01 (0.55)	0.00 (0.08)
	10	-0.10 (6.04)	0.09 (0.76)	0.04 (0.55)	0.00 (0.06)
	15	0.16 (4.83)	0.10 (0.74)	0.04 (0.55)	0.00 (0.07)
	20	0.30 (4.53)	0.10 (0.72)	0.03 (0.52)	0.00 (0.07)
3	ARL	1.23 (0.53)	1.18 (0.47)	1.13 (0.38)	1.03 (0.18)
	0	-10.45 (19.07)	-21.89 (29.70)	-8.72 (16.27)	-6.14 (10.83)
	5	0.04 (0.42)	-0.03 (0.48)	0.03 (0.33)	0.01 (0.15)
	10	0.04 (0.40)	-0.01 (0.43)	0.03 (0.31)	0.01 (0.15)
	15	0.06 (0.42)	-0.01 (0.40)	0.04 (0.31)	0.01 (0.15)
	20	0.05 (0.38)	-0.01 (0.42)	0.03 (0.31)	0.01 (0.14)

CHAPTER 4. RESEARCH 2.

Estimation of multiple change-points in time series normally distributed using a construction Heuristic and a Genetic Algorithm.

This is the second research about change-point analysis for independent observations normally distributed. It considers case when multiple step changes have occurred assuming that distribution's parameters as well as change-point positions are unknown. Maximum Likelihood estimators for change-points as well as for parameters were developed considering three cases based on single step change problem: (1) multiple changes only in the mean, (2) multiple changes only in variance and (3) multiple changes in both parameters at same time. Due to solve this problem leads to an optimization problem Construction Heuristic as well as a Genetic Algorithm (Evolutionary) were developed based on change-points MLEs. Comparison between these estimators was done in order to show their performance.

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Estimation of multiple change-points in time series Normally Distributed using a construction Heuristic and a Genetic Algorithm.

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Estimation of multiple change-points in a sequence of normal observations is a problem found in SPC. Frequently monitoring systems in statistical process control Phase I deals with situations where multiple change-points occur. Estimating these multiple change-points can be useful in the detection of assignable causes of variation in the process. In this research, maximum likelihood estimators of multiple change-points in a series of independent normal observations are derived for three cases: first one when multiple changes occurs only in the mean, second one when multiple changes occurs only in variance, and last one when multiple changes occur in both mean and variance. A combinatorial problem must be solved in order to find these multiple change-point estimators. For this reason a constructive heuristic and an evolutionary algorithm were developed to find these estimators. Performance analysis of maximum likelihood estimators and the heuristics mentioned previously is presented. Heuristics presented in this research present a similar behavior than the MLE.

Keywords: Change point analysis, maximum likelihood estimator, heuristic algorithm.

4.1. Introduction.

When monitoring a system, managers need tools to determine whether the process is under statistical control or not. In statistical process control (SPC), well known tools used are control charts, which are capable to detect if the process is under statistical control, but they are not capable of detecting the initial moment at which a sustained change occurred. Knowing this moment simplifies the search of assignable causes of variation. Change-point analysis is the methodology used to estimate the initial moment when processes get out of control. Estimators can be used with control charts in a sequential way for system management.

Change-point analysis started from a parametric approach with Hinkley (1970) who constructed maximum likelihood estimators (MLE) and likelihood ratio tests (LRT) for a change in the mean of a normal process with initial known parameters. Following this guideline, several authors like Samuel, Pignatiello and Calvin (1998) and Khoo (2004) have analyzed the behavior of MLE in normal time series for different scenarios. These estimators were developed assuming prior knowledge of parameters, i.e. in the Phase II of SPC. For case when there is no information of initial parameters in a normally distributed process, Phase I of SPC, Tercero et al. (2013a) developed the MLE for a change in mean and integrated this estimation with a self-starting cumulative sum control chart (CUSUM).

In Phase I of SPC is probably that multiple changes occur. Perry, Pignatiello, and Simpson (2007) mentioned that a process might have multiple step changes as a consequence of influential process input variables at different times. Amiri and Allahyari (2011) categorize the different changes types as step change, multiple step changes, drift change and monotonic change. Sullivan (2002) developed a multiple change-point estimator for the mean of a series using a clustering algorithm. Jann (2000) analyzed a time series with multiple changes in mean in a normal process and proposed an estimator of these multiple change points based on the t-test for shifts in mean. He also developed a genetic algorithm in order to deal with the non-polynomial time needed to obtain these estimators and used a cost function to estimate the number of changes in the series.

In this research multiple change-points MLEs of a normally distributed time series, where distribution parameters before and after each change are unknown, are derived. Also two heuristics are presented in order to find these estimators. This paper is organized as follows: Section 4.2 includes a literature review for change-point analysis. Section 4.3 presents the model and change-point and parameters MLE's derivation. In Section 4.4 two heuristics to solve the optimization problem for finding the multiple change-points MLEs are described. In Section 4.5 numerical experimentation is done in order to analyze the performance of the MLE and the two heuristics developed. Finally, in Section 4.6 conclusion and future work are presented.

4.2. Literature Review

The problem of detection of a change in a random process was analyzed first, from the Bayesian approach, by Girshick and Rubin (1952), who defined a quality control rule to trigger corrective actions when a change is detected. In the classical perspective, Page (1955) developed the cumulative sum control chart, CUSUM, to detect sustained changes based on SPC theory.

From parametric approach, Hinkley (1970) sets the theoretical foundations for constructing MLEs and LR tests to make inferences and estimate the change-point in a normally distributed time series with a shift in the mean in Phase II of SPC. Using these results, Samuel, Pignatiello, and Calvin (1998a); Samuel and Pignatiello (1998); Dabye and Kutoyants (2001); Pignatiello and Samuel (2001); Nedumaran, Pignatiello and Calvin (2002); Timmer and Pignatiello (2003); and Liming (2008) developed change-point MLEs for other distributions and different scenarios. Fotopoulos, Jandhyala and Khapalova (2010) derive an exact computable expression for the asymptotic distribution of the change-point MLE for normally distributed series. Most of these authors mainly work with the integration of change-point estimators with control charts.

Several tests to make inference about changes have been developed. Timmer, Pignatiello and Longnecker (1998) developed CUSUM chart based on LR test to detect changes in a AR(1) process. Hawkins and Zamba (2005a), proposed a model to deal with change in variance of a normal process the Generalized Likelihood Ratio (GLR) based on Bartlett's test in SPC Phase I. Later, Zamba and Hawkins (2006) developed and LR test for multivariate normal process; and Batsidis (2010) developed a LR test for multiple changes in mean in elliptical countoured distributions. Using GLR methodology and adding a moving window to simplify the approach, Reynolds and Jianying (2010) developed a GLR control chart for small shifts in the process mean. Later, Tercero et al. (2013b) constructed an estimator based on the p-value function of the Mood's median test for changes in the trend of Random Walk Models with Drift. For a detailed study of contributions of parametric approach, see Amiri and Allahyari (2011).

The estimation of multiple change-points in time series has been studied because of its applications which include meteorology, analysis on DNA sequences, signal processing, econometrics, and statistical process control. In climate data analysis change-point problem addresses a lack of stationary in a time series. Examples of researches in this area includes: Potter (1981), who used a likelihood ratio test for bivariate normal distribution developed by Maronna and Yohai (1978) and proposed the maximum of the likelihood ratio tests for all feasible cuts in a series as a statistic test for a single change; Easterling and Peterson (1995) proposed using a combination of regression analysis and nonparametric statistics for detecting inhomogeneities in a climatological time series; Lanzante (1996), developed a non-parametric iterative test based on the Wilcoxon-Mann-Whitney test for a single and multiple changes; and Alexandersson and Moberg (1997) created a normal standard homogeneity test for testing changes in trends and variances using a likelihood ratio test. On DNA sequence's analysis, Arunajadai (2009) presents a methodology to model the RNA unwinding mechanism by using Tukey's biweight function to detect changes in the mean. Fu and Curnow (1990) derived the MLE distribution of the location of two changed segments in a sequence of Bernoulli independent variables and applied their results to the prediction of protein helical regions.

Tests for multiple change points have been developed by several authors, like Huskova and Slaby (2001), who get approximations to the critical values for tests in location models; Aly, Abd-Raboun and Al-Kandari (2003) developed a test when the changes are in the same direction and present the asymptotic null distribution (of no changes) of that test. Jann (2000), developed a genetic algorithm to find the number and the estimation of multiple change-points in a normal series for shifts in the mean using a statistic based on t-test. Because of the complexity of analyze all possible combinations of changes the author proposed a genetic algorithm to find the multiple change-point estimators. He also used a cost function based on the mean of the cumulative associated Student's probability density function adding two parameters, one to reflects the wish of identifying potential change-points, i.e., it helps in determine the number of change-points; and a second one for separate the bit sequences which contains interesting positions of the change-points from those who look not have interesting change-point positions, in other words, helps to keep solutions that have potential change-points locations

This research derives multiple change-points MLEs in a process with observations normally distributed with changes in mean and/or variance in Phase I of SPC. Because of the complexity of analyze all possible combinations of multiple change-points in this research two heuristics procedures are developed and compared its performance with MLEs one using Monte Carlo simulation.

In the following Section MLE's derivation for multiple change-points when parameters, before and after changes, are unknown of normally distributed time series of independent observations is presented.

4.3. Model.

Suppose a normally distributed time series with m sustained changes in one or both of its parameters. Let T be the size of the time series of independent normal samples. Mathematically is expressed as follows:

$$X_{i} \sim \begin{cases} N(\mu_{1}, \sigma_{1}^{2}) & \text{if } 1 \leq i \leq \tau_{1} \\ N(\mu_{2}, \sigma_{2}^{2}) & \text{if } \tau_{1} < i \leq \tau_{2} \\ N(\mu_{3}, \sigma_{3}^{2}) & \text{if } \tau_{2} < i \leq \tau_{3} \\ \vdots \\ N(\mu_{m+1}, \sigma_{m+1}^{2}) & \text{if } \tau_{m} < i \leq T \end{cases}$$
(1)

where X_i is a vector of sampled observations size *n* and τ_k , k = 1,...,m, are the *m* unknown change-points. Also, suppose that parameters μ_k and σ_k^2 , k = 1,...,m,m+1 are unknown and then they have to be estimated.

In Subsections 4.3.1, 4.3.2 and 4.3.3 MLE's for unknown parameters in (1) and multiple change-points are derived using Hinkley's (1970) methodology for the following cases:

Case 1: In the time series m sustained changes occur only in the mean, while variance remains constant over the process, i.e.:

$$\mu_k \neq \mu_{k+1}; \ \sigma_1^2 = \sigma_2^2 = \dots = \sigma_{m+1}^2 = \sigma_p^2; \ \forall k = 1, 2, \dots, m.$$
 (2)

Case 2: *m* sustained changes occur only in variance, while mean of the process remains constant, i.e.:

$$\mu_{k} = \mu_{k+1} = \mu; \ \sigma_{k}^{2} \neq \sigma_{k+1}^{2}; \ \forall k = 1, 2, ..., m.$$
(3)

Case 3: In the time series m sustained changes occurred in both parameters, mean and variance. This case is the most general case because no assumption about the parameters is given; i.e.:

$$\mu_k \neq \mu_{k+1}; \ \sigma_k^2 \neq \sigma_{k+1}^2; \ \forall k = 1, 2, ..., m.$$
 (4)

4.3.1. Maximum Likelihood Estimators for shifts in the mean. Case 1.

Consider a process following (1) where *m* changes occur, each one at time τ_k for k = 1,...,m and variance remains constant over the process. Following Hinkley's (1970)

guideline maximum likelihood estimators for parameters and change-points are derived. The likelihood function for this scenario is:

$$L = \prod_{i=1}^{\tau_1} \prod_{j=1}^n f(x_{ij}, \mu_1, \sigma_p) \cdot \ldots \cdot \prod_{i=\tau_m+1}^T \prod_{j=1}^n f(x_{ij}, \mu_{m+1}, \sigma_p)$$
(5)

And so, the log likelihood function is:

$$\log L = -\frac{nT}{2} (\log(2\pi) + \log(\sigma_p^{(2)})) - \frac{1}{2\sigma_p^{(2)}} \left[\sum_{i=1}^{\tau_1} \sum_{j=1}^n (x_{ij} - \mu_1)^2 + \dots + \sum_{i=\tau_m+1}^T \sum_{j=1}^n (x_{ij} - \mu_{m+1})^2 \right]$$
(6)

MLEs for τ_r , μ_k and σ_p , r = 1,...,m, k = 1,...,m,m+1, are given by those values that maximizes (5) or (6). Mean and variance estimators for each subsection are presented in (7) and (8), respectively, using first order condition for optimality of (6).

$$\hat{\mu}_{k} = \frac{\sum_{i=\tau_{k-1}+1}^{\tau_{k}} \sum_{j=1}^{n} x_{ij}}{n(\tau_{k} - \tau_{k-1})} \quad \text{if} \quad 1 \le k \le m+1$$
(7)

$$\hat{\sigma}_{p}^{2} = \frac{\sum_{i=1}^{\tau_{1}} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{1})^{2} + \dots + \sum_{i=\tau_{m}+1}^{T} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{m+1})^{2}}{nT}$$
(8)

where $\tau_0 = 0$ and $\tau_{m+1} = T$.

Substituting (7) and (8) in (6), find τ_r , r = 1,...,m values which maximize (6), i.e., the multiple change-points MLEs are:

$$\hat{\tau} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \log(\hat{\sigma}_p^{-2}(\hat{\mu}_1, \hat{\mu}_2, \dots, \hat{\mu}_{m+1}))$$
(9)

or

$$\hat{\vec{\tau}} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \hat{\sigma}_p^2(\hat{\mu}_1, \hat{\mu}_2, \dots, \hat{\mu}_{m+1})$$
(10)

4.3.2. Estimators for multiple changes in variance. Case 2.

This case considers a series following (1) in which *m* changes occur in variance, but the mean over the process is the same. MLE for the common mean $\hat{\mu}$, and the variances $\hat{\sigma}_k^2$ of each sub-section as well as for the multiple change-points τ_r , r = 1, 2, ..., m, k = 1, 2, ..., m+1 are derived. The likelihood function (11) for this scenario is the following:

$$L = \prod_{i=1}^{\tau_1} \prod_{j=1}^n f(x_{ij}, \mu, \sigma_1^2) \cdot \ldots \cdot \prod_{i=\tau_m+1}^T \prod_{j=1}^n f(x_{ij}, \mu, \sigma_{m+1}^2)$$
(11)

Log-likelihood function is presented in (12):

$$\log L = -\frac{nT}{2}\log(2\pi) - \frac{n}{2}\sum_{k=1}^{m+1} (\tau_k - \tau_{k-1})\log(\sigma_k^2) - \frac{1}{2}\sum_{k=1}^{m+1}\sum_{i=\tau_{k-1}}^{\tau_k}\sum_{j=1}^n \frac{1}{\sigma_k^2} (x_{ij} - \mu)^2$$
(12)

where $\tau_0 = 0$ and $\tau_{m+1} = T$.

Applying first order condition of optimality, estimators of variances were found:

$$\hat{\sigma}_k^2 = \frac{\sum_{i=\tau_{k-1}+1}^{\tau_k} \sum_{j=1}^n (x_{ij} - \mu)^2}{n(\tau_k - \tau_{k-1})} \quad \text{if} \quad 1 \le k \le m+1$$
(13)

where $\tau_0 = 0$ and $\tau_{m+1} = T$.

The estimator of the process mean μ is obtained by solving the following equation for μ :

$$\frac{\sum_{i=1}^{\tau_1} \sum_{j=1}^n (x_{ij} - \mu)}{\sigma_1^2} + \frac{\sum_{i=\tau_1+1}^{\tau_2} \sum_{j=1}^n (x_{ij} - \mu)}{\sigma_2^2} + \dots + \frac{\sum_{i=\tau_m+1}^T \sum_{j=1}^n (x_{ij} - \mu)}{\sigma_{m+1}^2} = 0$$
(14)

It can be proved that solving (14) leads to find the roots of a polynomial of odd grade 2m+1, thus, it has at least one real root. If there are more than one real root, using those values and (13) in (12) to obtain the change-point MLEs:

$$\hat{\tau} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \left\{ \log \left(\hat{\sigma}_1^{\tau_1}(\hat{\mu}) \cdot \hat{\sigma}_2^{\tau_2 - \tau_1}(\hat{\mu}) \cdot \dots \cdot \hat{\sigma}_{m+1}^{T - \tau_m}(\hat{\mu}) \right) \right\}$$
(15)

This, (15), can also be written as:

$$\hat{\tau} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \left\{ \tau_1 \log(\sigma_1^2(\hat{\mu})) + (\tau_2 - \tau_1) \log(\sigma_2^2(\hat{\mu})) + \dots + (T - \tau_m) \log(\sigma_{m+1}^2(\hat{\mu})) \right\}$$
(16)

or:

$$\hat{\vec{\tau}} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \left\{ \hat{\sigma}_1^{\tau_1}(\hat{\mu}) \cdot \hat{\sigma}_2^{\tau_2 - \tau_1}(\hat{\mu}) \cdot \dots \cdot \hat{\sigma}_{m+1}^{T - \tau_m}(\hat{\mu}) \right\}$$
(17)

4.3.3. Estimators for Shifts in mean and variance. Case 3.

In this Subsection, m changes have occurred in both parameters at same time. MLEs for mean and variance in each subsection, as well as for multiple change-points are derived. Equation (18) presents the likelihood function for this scenario:

$$L = \prod_{i=1}^{\tau_1} \prod_{j=1}^n f(x_{ij}, \mu_1, \sigma_1^2) \cdot \dots \cdot \prod_{i=\tau_m+1}^T \prod_{j=1}^n f(x_{ij}, \mu_{m+1}, \sigma_{m+1}^2)$$
(18)

And so, the log likelihood function is (19):

$$\log L = -\frac{nT}{2}\log(2\pi) - \frac{n}{2}\sum_{k=1}^{m+1} (\tau_k - \tau_{k-1})\log(\sigma_k^2) - \frac{1}{2}\sum_{k=1}^{m+1}\sum_{i=\tau_{k-1}}^{\tau_k}\sum_{j=1}^n \frac{1}{\sigma_k^2} (x_{ij} - \mu_k)^2 \quad (19)$$

Applying first order conditions to find maximums, MLEs for mean and variance subsections were found:

$$\hat{\mu}_{k} = \frac{\sum_{i=\tau_{k-1}+1}^{\tau_{k}} \sum_{j=1}^{n} x_{ij}}{n(\tau_{k} - \tau_{k-1})} \quad if \quad 1 \le k \le m+1$$
(20)

$$\hat{\sigma}_{k}^{2} = \frac{\sum_{i=\tau_{k-1}+1}^{\tau_{k}} \sum_{j=1}^{n} (x_{ij} - \hat{\mu}_{k})^{2}}{n(\tau_{k} - \tau_{k-1})} \quad \text{if} \quad 1 \le k \le m+1$$
(21)

Substituting (20) and (21) in equation (19), change-point MLEs were found:

$$\hat{\tau} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \left\{ \log \left(\hat{\sigma}_1^{\tau_1}(\hat{\mu}_1) \cdot \hat{\sigma}_2^{\tau_2 - \tau_1}(\hat{\mu}_2) \cdot \dots \cdot \hat{\sigma}_{m+1}^{T - \tau_m}(\hat{\mu}_{m+1}) \right) \right\}$$
(22)

This can also be written as:

$$\hat{\tau} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \begin{cases} \tau_1 \log(\sigma_1^2(\mu_1)) + (\tau_2 - \tau_1) \log(\sigma_2^2(\mu_2)) + \dots \\ + (T - \tau_{m+1}) \log(\sigma_{m+1}^2(\mu_{m+1})) \end{cases}$$
(23)

or:

$$\hat{\tau} = \arg\min_{\{\tau_1, \tau_2, \dots, \tau_m\}} \left\{ \hat{\sigma}_1^{\tau_1}(\hat{\mu}_1) \cdot \hat{\sigma}_2^{\tau_2 - \tau_1}(\hat{\mu}_2) \cdot \dots \cdot \hat{\sigma}_{m+1}^{T - \tau_m}(\hat{\mu}_{m+1}) \right\}$$
(24)

In all scenarios described previously finding the change-points MLEs is a combinatorial problem with $\binom{T+k-p-pk}{k}$ number of possible change-points locations where p is the minimum data required to be between changes. Easterling and Peterson (1995) forced that at least five (p = 5) observations must occur between change-points for statistical reasons. Computation time of all possible solutions increases as either number of changes or size of the series increases in a non-polynomial (NP) way. In next Section, two heuristics are presented in order to assess this problem.

4.4. Heuristics.

Modern optimization problems tend to deal with the analysis of large sets of information. When exact algorithms cannot be developed, or their time for finding the optimal solution is unacceptable, it is sufficient to find an approximate solution. Heuristics algorithms are defined by Kokash (2005) as algorithms that either give nearly the exact solution or provide good solution not for all instances of the particular problem. Heuristics are optimization techniques which exploit the knowledge of a specific problem and which solution is not guaranteed to be the optimal solution. These methods are widely used when dealing with NP optimization problems.

In this Section two heuristcs were developed to find a near solution of the optimization problem of finding the MLE. The first one, described in Section 4.4.1, is a constructive greedy algorithm, which in each stage takes the solution with best objective function within a neighbourhood, until a feasible solution is found, see Laporte (1992). Second heuristic is

an evolutionary algorithm; which finds a solution based on the natural selection (survival of the fittest) in a set of feasible solutions, see Eiben and Smith (2004).

4.4.1 Greedy constructive heuristic

The main idea in this constructive algorithm is detect the "most likely" single change–point in each step. After detecting this change-point, greedy algorithm looks for the next single change-point looking for the "most likely" change-point in the two subsections, the first one between the initial point and the first change-point estimated and the second subsection between this change-point estimation and the last observation, choosing the value which minimizes log likelihood function for m = 2 as the second change-point. Greedy algorithm continues looking the "most likely" change point in each subsection and stops when mchange-points are estimated. Pseudo code of this algorithm is described below:

- 1. Name the fifth observation as T_0 and T-5 observation as T_1 , initialize i=1. (This restriction for T_0 and T_1 was explained in Section 4.3.3).
- 2. While $i \neq k$,
 - a. Estimate a change point in each subgroup $\{T_{j-1}, T_j\}$, for all $0 < j \le i$, looking the maximization of (10), (17) or (24), for cases 1, 2 or 3, respectively for m=1. Named each change-point found as t_j .
 - b. Let $P_j = \{T_1, ..., T_{i-1}, t_j\}$ and set $\vec{\tau}_j = \langle P_{j(r)} \rangle$ for $0 < r \le i$, where $P_{j(r)}$ is the order statistics of the sample P_j .
 - c. Select $\vec{\tau}^*$ between all $\vec{\tau_j}$ which optimizes (7), (14) or (21), for m = i
 - d. Rename $T_j = \overrightarrow{\tau}^*(j)$ for all $0 < j \le i$ and $T_{i+1} = T 5$. Do i = i+1.
 - e. End while.
- 3. Make $\vec{t}_C = \vec{\tau}^*$.

This heuristic will be compared with a stochastic algorithm described in next Section.

4.4.2 Evolutionary Heuristic

Evolutionary algorithms are based on the principles of the natural selection laws, which state that the fittest individuals are those who survive. The most common approach is focused on the following scheme: there is an objective function that is going to be optimized, then randomly generates a pool of solutions (called a population of individuals);
in order to classify the population, these solutions are evaluated in the objective function (measure of fitness) and the best ones are selected in order to be the seed of the following solutions' pool (next generation). New solutions are obtained by crossover and mutation. Crossover is the combination of two solutions (parents) to create one or more new solutions (children). The mutation is the process when a variation of an existing solution is made to create another individual. By these methods new solutions are added in the initial solutions' pool. Then, by some pre-set rules the remaining solutions (survivors) are selected, preserving the size of that pool. After repeating this procedure several times (generations) good quality solutions are found.

It is noteworthy that evolutionary algorithms manage a high level of stochasticity, which keeps diversity of the solutions' pool. Selection process needs to be such that the solutions' pool maintains the individuals with best objective function and few solutions with not so good fitness value. One of the main features of evolutionary algorithms is to be adapted to the environment in which the solutions are embedded. For this reason, every problem must have advantages and difficulties; therefore, evolutionary algorithms' scheme needs to consider the essential characteristics of each problem.

In this particular problem of finding multiple change-points, the evolutionary algorithm proposed omits the combination of solutions, because of it creates a high percentage of infeasible solutions (abortions). The diversity in the solution pool is maintained because of the randomness of the process and the number of selected tournaments for the selection part. Next the pseudo-code for the proposed algorithm is presented:

- 1. CREATION of the initial random population.
- 2. EVALUATION of the individuals.
- 3. While STOP CRITERION is unsatisfied.
 - 3.1 MUTATION to all individuals.
 - 3.2 EVALUATION of the mutations.
 - 3.3 SELECTION of the survivals.
- 4. End while.

The description of each stage of the algorithm implemented is described below:

- 1. The representation of a solution s_i is made by a vector of *k* components, where each component represents the position where a change occurred in the time series.
- 2. The initial population is created by generating N solution vectors with exactly k randomly changes, always ensuring the feasibility, this is, changes are located at least five observations separated. Generate P_0 , where $|P_0| = N$.
- 3. To evaluate the fitness of each individual's fitness function was necessary to evaluate function (10), (17) or (24), according to the case choose, which obtains the more probably change-points of the time series.
- 4. Mutation was applied to all the individuals, such that each individual always maintain its cardinality. Then, it was decided to only perform an exchange between components of the same solution. In this step we obtained P_m .
- 5. The selection step was carried out in an elitist way but being aware of keeping diversity, this is the reason for deciding to conduct a selection based on a tournament. It was considered P=P₀ ∪ P_m, where evidently |P| = 2N, and randomly selected two elements of this pool of solutions, that is, s_i, s_j ∈ P, where i ≠ j. Then, the fitness function F(·) was evaluated and these values were compared, if F(s_i) ≤ F(s_j) then W(s_i) = W(s_i)+1, where W(s_i) is the winner function associated to the i-th solution. Otherwise, if F(s_i) > F(s_j), then W(s_j)=W(s_j)+1. After a certain number of tournaments the N best individuals based on their W(·) were selected. If the number of tournaments held is not large, this criterion allows maintain diversity in the population.

Selected parameters for this algorithm, such as the number of generations, the population size and the number of tournaments were chosen based on numerical results.

4.5. Experimentation Design

As seen in Table 8, to evaluate change-point estimators' performance, several factors were considered. Over different scenarios, a sensitivity analysis was done by determining the effects on bias (mean error) and the standard error of the estimators.

Factors	Levels		
Estimators	$\hat{\tau}_{mle1}, \ \hat{\tau}_{mle2}, \ \hat{\tau}_{mle3}, \ \hat{\tau}_{EV1}, \hat{\tau}_{EV2}, \hat{\tau}_{EV3}, \\ \hat{\tau}_{C1}, \hat{\tau}_{C2}, \hat{\tau}_{C3}$		
Number of changes (<i>k</i>)	2, 3, 4		
Shift in the mean (δ)	2σ, 1σ (k=2) 2σ, 1σ, -3σ (k=3) 2σ, 1σ, -3σ, 1σ (k=4)		
Ratio of deviations (σ_k / σ_{k-1})	2, 1.5 (k=2) 2,1.5,0.5 (k=3) 2,1.5,0.5,2 (k=4)		
Series length (T)	300, 900, 1500		
Change-point position (τ/T)	1/3, 2/3 (k=2) 1/4, 2/4, 3/4 (k=3) 1/5, 2/5, 3/5, 4/5 (k=4)		

Table 8. Factor to measure the performance of change-point estimation

Monte Carlo experimentation was used to evaluate the performance of the change-point estimators. The following general procedure was used for each scenario under evaluation:

- 1. Select the scenario from Table 8.
- 2. Generate T random variables according to the selected scenario.
- 3. Estimate the change-point $\hat{\tau}$ (using estimators under analysis).
- 4. Repeat step 2 and 3 10,000 times.
- 5. Calculate the mean and standard deviation of $\vec{\tau} \hat{\vec{\tau}}$.
- 6. Calculate the average time to get estimations.
- 7. Calculate performance of MLE, when it is feasible, and heuristics.
- 8. Return to step 1 and select another scenario.

10,000 replicates in step 2 ensure that standard deviation of mean change-point $\hat{\tau}$ is reduced 100 times. Results of the experimentation are resumed in Tables 9, 10 and 11. $\hat{\tau}_{MLEi}$ for i = 1,2,3 was obtained over all possible combinations. Due to the computational time required for obtaining these values and the number of simulations, estimations only were computed for k = 2. Performance of estimators is shown in Tables 9, 10 and 11 which corresponds to k values of 2, 3 and 4, respectively.

Table 9. Performance of multiple change-point estimators for k = 2 changes.

Performance of $\hat{\tau}_{EV}$ and $\hat{\tau}_{C}$ were evaluated over different cases (1,2,3), and size of the series according to Table 1 for k = 2. Estimations are presented next to their corresponding standard error, which are within parentheses. Solving time (ST) is presented (in secs.).

$k=2$ $\hat{\tau}_{_{MLE}}$		$\hat{ au}_{\scriptscriptstyle EV}$			$\hat{\tau}_{_C}$					
Case		T=300	T=900	T=1500	T=300	T=900	T=1500	T=300	T=900	T=1500
	ĉ	0.01	0.01	0.00	0.02	0.00	0.00	-0.42	-0.54	-0.54
	ι_1	(1.28)	(1.24)	(1.27)	(1.29)	(1.30)	(1.47)	(1.84)	(1.74)	(1.67)
1	ŕ	0.08	0.02	-0.02	0.08	0.07	-0.03	0.00	0.01	-0.09
	<i>t</i> ₂	(6.04)	(5.36)	(4.99)	(6.04)	(5.41)	(5.40)	(5.95)	(5.36)	(5.01)
	ST	3.11	30.11	88.85	0.90	0.93	0.98	0.02	0.08	0.14
	$\hat{\tau}$	0.06	-1.51	-1.61	0.44	-1.42	-1.38	-2.36	-4.31	-4.16
	ι,	(11.72)	(5.71)	(5.72)	(13.47)	(5.75)	(5.86)	(13.00)	(8.75)	(8.23)
2	÷.	÷-1.38	-3.46	-3.23	-0.34	-3.35	-2.86	-1.23	-3.42	-3.35
	<i>t</i> ₂	(25.31)	(17.98)	(16.92)	(28.38)	(18.42)	(17.07)	(25.66)	(18.96)	(17.18)
	ST	2.15	23.90	77.63	0.98	1.07	1.20	0.02	0.11	0.22
	$\hat{\tau}$	-0.14	-0.53	-0.55	0.41	-0.48	-0.33	-0.59	-0.92	-0.88
3	ι_1	(5.69)	(1.99)	(1.96)	(9.29)	(2.02)	(1.06)	(5.81)	(2.18)	(2.08)
	\hat{t}_2	-1.16	-2.37	-2.50	0.71	-2.19	-1.96	-1.51	-2.41	-2.51
		(19.38)	(11.53)	(11.73)	(26.11)	(11.63)	(11.84)	(18.74)	(11.54)	(11.71)
	ST	3.01	31.80	97.66	1.08	1.19	1.33	0.03	0.10	0.18

Table 10. Performance of heuristics for multiple change-point estimators for k = 3 changes.

Performance of $\hat{\tau}_{EV}$ and $\hat{\tau}_{C}$ were evaluated over different cases (1,2,3), and size of the series according to Table 1 for k = 3. Estimations are presented next to their corresponding standard error, which are within parentheses. Solving time (ST) is presented (in secs.).

k	= 3		$\hat{ au}_{\scriptscriptstyle EV}$			$\hat{ au}_{C}$	
Case		T=300	T=900	T=1500	T=300	T=900	T=1500
	$\hat{ au}_1$	0.00	-0.03	-0.08	-0.17	-0.13	-0.13
		(1.36)	(1.73)	(2.24)	(1.76)	(1.65)	(1.71)
	$\hat{\tau}_2$	-0.17	-0.16	-0.03	-0.20	-0.12	-0.08
1		(6.47)	(6.45)	(7.56)	(7.03)	(5.46)	(5.35)
	ĉ	0.00	-0.03	-0.03	-0.28	-0.29	-0.31
	<i>L</i> ₃	(1.14)	(0.81)	(1.16)	(0.92)	(0.92)	(0.97)
	ST	1.17	1.18	1.22	0.04	0.12	0.20
	$\hat{ au}_1$	0.53	-1.14	-0.82	-0.73	-1.98	-1.62
		(13.26)	(8.35)	(7.40)	(13.39)	(15.14)	(19.72)
	$\hat{\tau}_2$	-6.27	-3.06	-2.00	-6.48	-6.11	-4.95
2		(31.11)	(25.81)	(27.70)	(31.35)	(42.90)	(52.83)
	$\hat{ au}_3$	-0.42	0.95	-0.48	-3.17	-2.51	-2.03
		(12.90)	(8.01)	(8.04)	(14.00)	(20.25)	(22.42)
	ST	1.55	1.61	1.75	0.05	0.15	0.29
3	$\hat{ au}_1$	0.94	-0.21	0.18	0.18	-0.61	-0.55
		(9.73)	(3.13)	(2.51)	(6.67)	(2.03)	(2.01)
	t ₂	-2.39	-1.61	-0.88	-2.24	-2.40	-2.30
		(32.07)	(13.56)	(13.04)	(22.57)	(12.16)	(11.84)
	$\hat{ au}_3$	-1.18	0.15	-0.20	-0.59	0.25	0.29
		(10.53)	(3.81)	(2.59)	(7.00)	(1.99)	(2.11)
	ST	1.32	1.49	1.53	0.04	0.13	0.25

Table 11. Performance of heuristics for multiple change-point estimators for k = 4 changes.

Performance of $\hat{\tau}_{EV}$ and $\hat{\tau}_{C}$ were evaluated over different cases (1,2,3), and size of the series according to Table 1 for k = 4. Estimations are presented next to their corresponding standard error, which are within parentheses. Solving time (ST) is presented (in secs.).

<i>k</i> = 4			$\hat{ au}_{\scriptscriptstyle EV}$		$\hat{ au}_{C}$		
Case		T=300	T=900	T=1500	T=300	T=900	T=1500
	$\hat{ au}_1$	0.01	-0.03	-0.08	0.03	0.20	0.25
		(1.84)	(1.93)	(2.64)	(2.08)	(1.79)	(1.81)
	$\hat{\tau}_2$	0.00	0.08	0.02	0.06	-0.05	0.04
		(7.32)	(7.17)	(8.59)	(6.99)	(5.59)	(5.30)
1	<u> </u>	0.01	0.00	0.02	-0.06	-0.05	-0.04
	\mathcal{I}_3	(2.66)	(0.95)	(1.39)	(1.97)	(0.57)	(0.58)
	â	0.16	-0.14	-0.04	0.17	-0.04	0.00
	$ au_4$	(7.02)	(6.91)	(8.56)	(6.88)	(5.70)	(5.26)
	ST	1.32	1.33	1.42	0.04	0.15	0.26
	â	1.11	-0.93	-0.56	0.87	-3.38	-3.70
	ι_1	(13.90)	(8.28)	(6.76)	(15.49)	(12.16)	(11.32)
	t ₂	-7.33	-3.18	-1.74	-0.76	-8.91	-7.07
		(33.05)	(23.89)	(20.71)	(36.15)	(46.33)	(48.09)
2	$\hat{ au}_3$	-3.82	0.44	-0.11	-2.24	-3.99	-2.14
		(21.29)	(9.84)	(8.63)	(34.40)	(43.39)	(47.52)
	$\hat{ au}_4$	-2.20	-0.88	-0.27	-4.76	-10.15	-11.54
		(14.68)	(7.73)	(7.27)	(26.98)	(27.09)	(30.63)
	ST	1.53	1.60	1.69	0.06	0.20	0.37
	$\hat{ au}_1$	1.16	-0.04	0.54	0.45	-0.65	-0.62
3		(9.41)	(3.06)	(3.08)	(7.17)	(2.04)	(2.09)
	\hat{t}_2	-7.42	-1.47	-0.04	-4.89	-3.30	-2.55
		(33.25)	(16.00)	(14.38)	(24.45)	(16.56)	(13.68)
	$\hat{ au}_3$	-6.23	-0.22	-0.66	-1.45	1.41	1.46
		(20.76)	(5.42)	(2.99)	(13.38)	(3.34)	(3.32)
	$\hat{\tau}$	-1.96	-0.33	0.47	-2.36	-1.44	-1.34
	ι ₄	(13.00)	(6.02)	(6.25)	(9.99)	(5.03)	(4.77)
	ST	1.64	1.71	1.80	0.06	0.18	0.32

On all evaluated scenarios, time of simulations made with Constructive Algorithm's were less than 0.38 seconds while Evolutionary's ones were less than 1.80 seconds. For k = 2, tables shows that Evolutionary algorithm has more accuracy to MLEs estimations than Constructive.

When $k \neq 2$, when there are only k shifts in the mean, performance of both algorithms is similar with differences of biases less than ± 0.6 . For only k changes in ratio of deviations, Constructive shows bigger bias and standard error in almost all scenarios and its standard error increases as T increases while Evolutionary's bias and standard error decreases. Finally, when k changes occur in both parameters, Constructive has smaller bias and standard error when T = 300, if T>300 its bias are greater than Evolutionary.

4.6. Example: measuring the length of a laser scanned object

Laser scanners are useful tools to measure morphologies quickly and precisely. Sometimes it is necessary to use the data from the scanned object to measure its length. Figure 3 show a profile of 1024 measurements from a "flat" object that was positioned over the scanner table. There are two change points; the first one corresponds to the moment when measurements change table to object and the second change-point when measurements change from object to table. To measure the length of the object, the position of the two change points has to be determined in order to calculate the distance between them.



Figure 3. A profile of an object using a scanner laser with two change-points.

A profile of an object is obtained using a laser scanner. Two change-points are estimated to obtain an automatic measurement of the length of the object. Change-points indicated with dotted lines corresponds to the ones estimated using the exact MLE. Change points are estimated using estimators $\hat{\tau}_{mle1}$, $\hat{\tau}_{c1}$, and $\hat{\tau}_{EV1}$. Results from these estimations are shown in

Table 12. Using the laser scanner data, change-points are estimated using the three methods for situations when a change occurred only in the location parameter.

Estimation Mathad	Observation number of	Observation number of		
Estimation Method	the first change-point	the second change-point		
Exact MLE ($\hat{\tau}_{mle1}$)	345	749		
Constructive heuristic ($\hat{\tau}_{c1}$)	345	749		
Evolutionary heuristic ($\hat{\tau}_{EV1}$)	344	749		

Table 12. Change-point estimations for a series with 2 changes in the mean. Numerical example.

A change-point estimated at observation 345 indicates that a change occurred between observations 345 and 346, which is translated into positions -12.055 and -11.745 millimeters, giving a midpoint of -11.9 millimeters. The second change-point was estimated between observations 749 and 750, which gives positions 13.465 and 14.06 millimeters, giving a midpoint of 13.7625. The length of the scanned morphology is calculated by subtracting the second change-point minus the first change-point. A length of 25.6625 millimeters is measured.

4.7. Conclusions

MLEs computation time increases in a non-polynomial way as sizes of series and number of changes increases. Results show that Constructive Algorithm estimations are obtained quickly, but they are less accurate to corresponding MLEs than Evolutionary Algorithm estimations (in cases which they could be compared) which require less than 2 seconds to be done. Also, the latter ones are more consistent while Constructive presents a variation which depends of the case chosen. For future work, an integration of a local search to Constructive Algorithm will be done, as well as an integration of Evolutionary and Constructive algorithms. Because in real life it is difficult have a priori knowledge of the exact number of changes, this assumption could be discarded by using the CUSUM technique. Hypothesis test and confidence intervals will be developed to determine if the change(s) detected are significant or not and have a bind region for it (them).

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CHAPTER 5. CONCLUSIONS AND FUTURE WORK.

5.1. General conclusions.

This section summarized the state of art of the research. After that, remark the differences between assumptions and solution approaches of this research and the others found in literature. Contributions provided by this research are described in section 5.2 and future work in Section 5.3. This research addresses the change-point problem which generally speaking could be stated as question mentioned in section 1.2: Are the data homogeneous and if not, what are the locations of the homogeneous segments in the data? (Arunajadai, 2009, p.58). These locations are called change-points and finding them in Change-point Analysis (CPA) is the main duty.

This research is divided in two main works, which deals with the problem of estimation of change-points in a time series of independent normal observations. In next paragraphs they were explained.

First one was focused on developing change-point MLEs for independent and normally distributed observations when parameters (before and after the change) are unknown. In addition, the evaluation of their performance in a retrospective analysis and a comparison with change-point estimators found in literature was performed. Finally, the integration with Q-charts was also performed to show their performance in on-line monitoring. Comparison was performed by exhaustive simulation, considering different sample size (50, 100, 300, 1000), subgroup size (1, 3, 5), change-point locations (at quantiles 0.2, 0.3, 0.5), shifts in the mean (σ , 1.5 σ , 3 σ), and change in variance (1.3, 1.5, 3). Results show that MLE for shifts in the mean is robust to change-point location.

Second research was focused on developing multiple change-point MLEs for normally distributed series and heuristics because according to Jann (2000, p.68) "it is found imperative to treat the problem of multiple change-point detection as one of global

optimization". Additionally, an evaluation of their performance was performed. This evaluation was performed considering different sample sizes (300, 900, 1500), number of changes k (2, 3, 4) and considering change-point locations at every T * i/(k+1) for i = 1,2,...k. Results suggest that Evolutionary Algorithm is more precise than Constructive Algorithm to MLEs estimations.

Even though there are change-points MLEs in literature for simple step change-point problem, its derivation supposes knowledge about initial parameters. On the other hand, there are change-point estimators which do not assume that, but they do not correspond to MLEs.

5.2. Findings from this research.

In order to summarize conclusions of this research, they are divided for each of the hypothesis made in Chapter I.

- Conclusion of H.1: It is possible to develop change-point MLEs for both single and multiple changes when there is not prior knowledge about parameters. These estimators were found considering independent normally distributed observations, and discrete time. That is to say, it is possible to find parameters values that maximized Likelihood Function even with discrete time.
- Conclusion of H.1.1.: Considering separately three cases addresses, (1) for change only in mean results show that both estimators perform alike in means of bias, but CUSUM estimator has less spread when change-point location is in the middle of the series. Nevertheless, change-point MLE is more robust to the change-point location; (2) when there is only change in variance, both estimators perform alike in means of bias and spread, but Hawkins' estimator requires less operations to be obtained due to avoid the problem of obtain roots of a polynomial of degree higher than 2; and (3) for change in both mean and variance, CUSUM and Hawkins' change-point estimators tends to have smaller bias and spread than MLE when there is only change in mean, and only in variance, respectively. However, MLE

improves its precision as magnitude of the change increases for such cases. For cases with both changes, MLE perform better in means of bias and spread.

- Conclusion of H.1.2.: Results suggest (as expected) that change-point MLEs bias and spread decreases as the size of the series and as the number of replicates increases in all cases.
- Conclusion of H.1.3.: Tables 5 and 6 show that when Q-charts' ARL is larger, then MLE spread and bias is smaller, except maybe for cases of small samples size. In the other hand, when Q-charts' ARL is smaller, then MLE spread and bias is larger. Nevertheless, letting the process run 5 extra observations MLE performance improves for both situations.
- Conclusion of H.2.1.: Finding the multiple change-point MLEs in multiple changes leads to an optimization problem due to there are $\binom{T+k-p-pk}{k}$ different

combinations which have to be compared in order to find them which make the time increase in a non-polynomial way as the number of changes increases. Thus, it is necessary to develop heuristics in order to address this problem.

- Conclusion of H.2.2.: Change-point MLEs and Evolutionary algorithms tend to have smaller bias than Constructive Algorithm.
- Conclusion of H.2.3.: Results for cases when it was possible to make a comparison (only 2 changes), Evolutionary Algorithm tends to be closer than Constructive from the MLEs estimations. Nevertheless, make one simulation of Evolutionary along all cases lies between 0.1 and 1.8 seconds, while Constructive is always less than 0.38 seconds for cases considered here.

It is noteworthy that:

- Procedure for obtaining the change-point MLEs (single or multiple) was reduced to a minimization of variances problem. There is scarce (if not no) results in literature that show this estimation problem in this way.
- For case of change only in variance, the derivation of the mean MLE leads always to a problem of finding the roots of a polynomial of degree 2k + 1 where k is the

number of change-point supposed in the series. For every series and every feasible point of estimation, this polynomial must be obtained.

• Change-point MLEs for multiple change-points requires an exhaustive number of comparisons and operations in each comparison. Actual computer resources do not allow us to make more extensive studies.

H.2.2. is not completely accepted as true since multiple change-point problem add one more factor to the design of the experiment proposed for single change-point problem making it more complex for obtaining solutions and making comparisons and in this research only a few scenarios were considered. H.2.3. also could not be taken as true; we stated that Evolutionary Algorithm tends to behave similar to MLE, but it only was proved over few scenarios. Finally, integration with Q-charts gives to managers a procedure to ensure a state of control, which could reduce costs of inspection and rejections.

5.3. Future Work.

This research was focused mainly on the development of change-points MLEs and evaluation of their performance letting as a future work:

- Development of hypothesis test for change-point in time series.
- Development of confidence intervals for the change-point estimation. In order to do this is necessary development of hypothesis tests.
- Consider series with trend, which in practice could represent the time at which a machine wears out.
- Consider auto correlate series.
- Comparison between Jann's (2000) algorithm and Heuristics presented here by means of bias and spread.
- Improve Constructive Algorithm by adding a local search or make an integration of both heuristics.
- Development of these tools from a nonparametric approach.

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