

A ROBUST ESTIMATION METHOD OF LOCATION AND SCALE WITH
APPLICATION IN MONITORING PROCESS VARIABILITY

ROHAYU BT MOHD SALLEH

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Universiti Teknologi Malaysia

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This thesis is dedicated to Pak Salleh and Mak Yam for their loves,
endless support and encouragement.



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ABSTRACT

This thesis consists of two parts; theoretical and application. The first part proposes the development of a new method for robust estimation of location and scale, in data concentration step (C-step), of the most widely used method known as fast minimum covariance determinant (FMCD). This new method is as effective as FMCD and minimum vector variance (MVV) but with lower computational complexity. In FMCD, the optimality criterion of C-step is still quite cumbersome if the number of variables p is large because of the computation of sample generalized variance. This is the reason why MVV has been introduced. The computational complexity of the C-step in FMCD is of order $O(p^3)$ while MVV is $O(p^2)$. This is a significant improvement especially for the case when p is large. In this case, although MVV is faster than FMCD, it is still time consuming. Thus, this is the principal motivation of this thesis, that is, to find another optimal criterion which is of far higher computational efficiency. In this study, two other different optimal criteria which will be able to reduce the running time of C-step is proposed. These criteria are (i) the covariance matrix equality and (ii) index set equality. Both criteria do not require any statistical computations, including the generalized variance in FMCD and vector variance in MVV. Since only a logical test is needed, the computational complexities of the C-step are of order $O(p \ln p)$. The second part is the application of the proposed criteria in robust Phase I operation of multivariate process variability based on individual observations. Besides that, to construct a more sensitive Phase II operation, both Wilks' W statistic and Djauhari's F statistic are used. Both statistics have different distributions and is used to measure the effect of an additional observation on covariance structure.

ABSTRAK

Tesis ini mengandungi dua bahagian; teori dan aplikasi. Bahagian pertama mencadangkan pembangunan kaedah baru untuk penganggaran teguh lokasi dan skala, dalam langkah penumpuan data (C-langkah), dari kaedah yang paling digunakan secara meluas dikenali sebagai penentu kovarians minimum cepat (FMCD). Kaedah baru ini efektif seperti FMCD dan varians vektor minimum (MVV) tetapi kerumitan pengiraannya adalah rendah. Dalam FMCD, secara optimum kriteria bagi C-langkah masih agak rumit jika bilangan pembolehubah p adalah besar disebabkan pengiraan sampel varians teritlak. Inilah alasan mengapa MVV diperkenalkan. Kerumitan pengiraan C-langkah dalam FMCD adalah peringkat $O(p^3)$ manakala MVV adalah $O(p^2)$. Ini adalah satu peningkatan yang bererti terutamanya untuk kes bila p besar. Dalam kes ini, walaupun MVV lebih cepat daripada FMCD, pengiraannya masih mengambil masa. Oleh itu, motivasi utama tesis ini ialah untuk mencari kriteria optimum yang lain dimana pengiraannya jauh lebih efisien. Dalam kajian ini, dua kriteria optimum yang berbeza yang boleh mengurangkan masa pengiraan di dalam C-langkah dicadangkan. Kriteria tersebut adalah (i) kesaksamaan kovarians matrik dan (ii) kesaksamaan set indeks. Kedua-dua kriteria ini tidak memerlukan sebarang pengiraan statistik, termasuklah varians teritlak dalam FMCD dan varians vektor dalam MVV. Disebabkan hanya ujian logik diperlukan, kerumitan pengiraan bagi C-langkah adalah peringkat $O(p \ln p)$. Bahagian kedua adalah penggunaan kriteria yang dicadangkan dalam Fasa I dalam pemantauan kepelbagaian proses multivariat secara teguh berdasarkan sampel individu. Selain itu, untuk membina operasi Fasa II yang lebih sensitif, kedua-dua statistik W daripada Wilks dan statistik F daripada Djauhari digunakan. Kedua-dua statistik mempunyai taburan yang berbeza dan digunakan untuk mengukur kesan penambahan data pada struktur kovarians.

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CHAPTER 1

INTRODUCTION

The aim of this chapter is to introduce the importance of this research. In Section 1.1, the background of the problem will be discussed followed by the statement of problem in Section 1.2. In the section which follows, the research objective and problem formulation will be presented. The scope of the study, thesis organization and the contribution of the study will be presented in Section 1.4, Section 1.5 and Section 1.6, respectively.

1.1 Background of the Problem

There is a quantum leap in modern manufacturing industries when ‘surpass customer expectation’ becomes a philosophy of quality since late 1990s. Industries believe that the importance to stay competitive is by producing not only high quality of process and products but also a creative, innovative and useful with pleasing unexpected features (Djauhari, 2011a). However, those criteria are not likely to be static, and will certainly be changed based on time and demands.

In practice, a fundamental idea to improve the quality of process and products is realized by reducing the process variability. Philosophically, process quality is the reciprocal of process variability. If the process variability is small then the quality will be high and the larger the process variability the lower the quality. Alt and Smith (1988) and Montgomery (2005) mentioned that monitoring process variability is as

important as monitoring the process mean. However, the effort to manage the process variability is far harder than managing the process mean or, equivalently, process level.

Since the customer demands become more and more complex, the term quality must be considered as a complex system. Statistically, this means that quality is a multivariate entity. Consequently, process quality monitoring must be in multivariate setting. Practically, the quality of the production process is determined by several quality characteristics, of which some or all are correlated. Therefore, since the correlations among characteristics must be taken into consideration, it is not allowed to control each characteristic individually.

In multivariate setting, one of the most widely used control methods and procedures to monitor the process level is based on Hotelling's T^2 -statistic. The advantages of this method are (i) this statistic is powerful tool useful in detecting subtle system changes (Mason and Young, 2001), (ii) relatively easy to use (Djauhari, 2005), (iii) appealing to practitioners because of its similarity to Shewhart type charts (Prins and Mader, 1997), (iv) reasonable approach (Sullivan and Woodall, 1996) and, (v) T^2 is an optimal test statistic for detecting a general shift in the process mean vector (Mason *et al.*, 1995).

However, as T^2 -statistic is a multivariate generalization of student t -statistic, that multivariate control charting method is only focusing on detecting the shift in the mean vector. Nevertheless, it has received considerable attention. See for example, Tracy *et al.* (1992), Wierda (1994), Sullivan and Woodall (1996), Woodall and Montgomery (1999), Mason and Young (2001, 2002), and Mason *et al.* (1995, 1996, 1997, 2003, 2011). In contrast, multivariate process variability monitoring had received far less attention in literature especially for individual observations compared to the case where monitoring is based on subgroup observations. The general idea of the former monitoring process can be seen, for example, in Sullivan and Woodall (1996), Khoo and Quah (2003), Huwang *et al.* (2007), Mason *et al.* (2009, 2010) and Djauhari (2010, 2011b). This is the reason why our focus in this thesis is on monitoring process variability based on individual observations.

In univariate setting, as can be found in any standard book of statistical process control, when only one quality characteristic is involved, process variability is monitored by using MR , R , S or S^2 control charts. But, when the number of quality characteristics, p , is more than one and the correlations among them are to be considered, then a multivariate chart is required. There is a great potential for misleading results if univariate chart is used for each characteristics especially of receiving a false alarm or not receiving a signal when the multivariate process is out-of-control. This is illustrated in Figure 1.1, where two quality characteristics that are positively correlated are monitored individually. In that figure, LCL_i and UCL_i are the lower control limit and upper control limit for the i -th characteristics; $i = 1, 2$. Horizontal axis is for the first characteristic while the vertical axis is for the second.

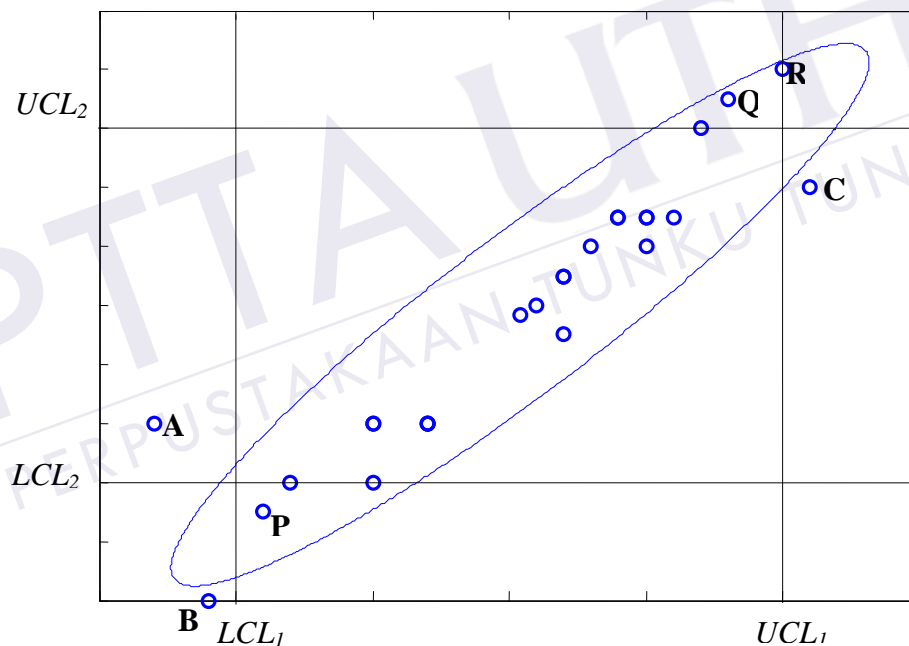


Figure 1.1 Elliptical control region versus rectangular control region

A few points inside the ellipse are in the state of in-control even though they are detected as out-of-control by using univariate chart for each characteristic. There are also three points A, B and C outside the rectangular control region and ellipse control region, representing significant out-of-control. However, univariate charts can easily fail to detect the potential signal. See the points P, Q and R. This is the danger of monitoring multiple correlated quality characteristics in univariate way.

Controlling all characteristics one by one is not allowed because of their correlations. Therefore, the requirement to monitor all characteristics simultaneously is demanded in current manufacturing industries. See also Montgomery (2005), Mason and Young (2002) and Ryan (2011) for further discussions.

Construction of control chart generally carried out in two phases; Phase I and Phase II. Phase I is a cleaning process of historical data set (HDS); abnormal or outlier data points examined and remove from the HDS to obtain the reference sample (RS). The existence of those data points may be caused by tools, machines, or human errors. Based on classical method as explained in Tracy *et al.* (1992), Wierda (1994), and Mason and Young (2001), any data points that lies beyond the control limits is removed after investigation for cause; otherwise they are retained. The process is continued until a homogeneous data set is obtained. This data set becomes the RS and provides the estimates of location and scale to be used for monitoring future observations in Phase II.

In practice, there is a certain situation in Phase I operation where outliers are undetected. It is because the use of classical method, i.e., Hotelling's T^2 statistic, is powerful when there is only one outlier exist (Hadi, 1992) but as explained by Sullivan and Woodall (1996, 1998), Vargas (2003) and Yanez *et al.*, (2010), it will performs poorly when multiple outliers are present. This latter situation as explained by Rousseeuw and van Zomeren (1990, 1991), Hadi (1992), Vargas (2003), Hubert *et al.* (2008) and Hadi *et al.* (2009) is usually due to masking and or swamping problems. In masking problem, outliers are considered as clean data points. Conversely, in swamping problem, clean data points are declared as outliers.

Chenouri *et al.* (2009) mentioned that the assumption that the Phase I data come from an in-control process is not always valid whereas Phase I is critical for the success of the actual monitoring phase. Therefore, successful Phase II depends absolutely on the availability of RS, to estimate location and scale parameters, obtained from HDS in Phase I operation. Since classical estimates of location and scale can be very badly influenced by outliers even by a single one, effort to address this problem is focused on estimators that are robust. Robust estimators are resistant

against the presence of outliers. Robustness of estimators is often measured by the breakdown point (BP) introduced by Donoho and Huber (1983). Maronna *et al.* (2006) defined the BP of an estimate $\hat{\theta}$ of the parameter θ is the largest amount of contamination such that the data still give information about θ . The higher the BP of an estimator, the more robust it is against outliers. The BP of the classical estimates is $\frac{1}{n}$ which means that even one outlier will ruin the estimates.

There are many different robust estimation methods for location and scale. The most popular and widely used high breakdown robust parameter estimation method is the so-called Fast Minimum Covariance Determinant (FMCD). It has the properties that the estimates are of high degree of robustness, has bounded influence function which ensures that the presence of outliers can only have a small effect on an estimator, and affine equivariant which ensures that any affine transformation does not affect the degree of its robustness.

As mentioned by Neykov *et al.* (2012), a recent development known as Minimum Vector Variance (MVV) has been introduced by Herwindiati *et al.* (2007). It is a refinement of data concentration step in FMCD developed for computational need. Meanwhile, Wilcox (2012) described MVV as a variation of the MCD estimator that searches for the subset of the data that minimizes the trace of the corresponding covariance matrix rather than determinant. However, it should be written as follows ‘minimizes the trace of squared of the covariance matrix’. Both FMCD and MVV consists of two steps; (i) to order p dimensional data points, $p > 1$, in the sense of centre-outward ordering, and (ii) to find the most concentrated data subset, called MCD set in the literature.

If FMCD uses “minimizing covariance determinant” as the optimal criterion in the second step, MVV uses “minimizing vector variance”. Interestingly, both FMCD and MVV produce the same robust Mahalanobis squared distance, i.e., the same MCD set, but with different computational complexity. The computational complexity of covariance determinant in FMCD is $O(p^3)$ while that of vector

variance is only $O(p^2)$. Although MVV gives a significant improvement in terms of computational efficiency (Herwindiati *et al*, 2007), the optimal criterion is still superfluous because covariance matrix is symmetric, each upper (or lower) diagonal element is computed twice. Furthermore, our simulation experiments show that the minimum of vector variance could be attained long before the convergence is reached. Therefore, specifically, in terms of computational efficiency, there is a need to find another criterion which ensures the faster running time. This is the first challenging problem that concerns Phase I operation.

On the other hand, concerning Phase II operation, most researchers are focused on monitoring process variability without passing through Phase I operation. This means that the initial covariance matrix Σ_0 is known which is not always the case in practice. There are very limited studies that concern on the case where Σ_0 is unknown which means that Phase I operation is a must to determine RS and estimate Σ_0 . Those who are working in this case are Mason *et al*. (2009) who used Wilks' W statistic and Djauhari (2010, 2011b) who proposed squared of Frobenius norm F statistic to monitor process variability in Phase II. Since, these statistics are defined to measure the effect of an additional observation on covariance structure based on different tools, they cannot be used individually. This is the second challenging problem that concerns Phase II operation to construct more sensitive monitoring procedure.

1.2 Problem Statement

Research background presented in the previous section leads us to the following research problems in robust monitoring process variability based on individual observations:

In Phase I operation:

- i. Develop a high breakdown point robust estimation method of location and scale giving the same robust Mahalanobis distance as FMCD and MVV but with lower computational complexity.
- ii. Construct a tool for multivariate normality testing.

In Phase II operation:

- i. Construct a more sensitive Phase II operation by using both Wilks' W statistic and Djauhari's F statistic separately.
- ii. Construct a tool to identify the root causes of an out-of-control signal, i.e., to identify which quality characteristics that contribute in that signal.

1.3 Research Objective and Problem Formulation

This thesis consists of two parts: theoretical and application. The principal objective of the first part is to find a better optimal criterion with lower computational complexity and giving the same result as FMCD and MVV.

The second part is the application of the proposed criterion in monitoring multivariate process variability based on individual observations. To achieve that, the main objective is to construct a control procedure that combine

- i. the high breakdown point robust location and scale estimates in the Phase I operation based on the proposed criterion
- ii. a more sensitive Phase II operation.

More specifically, in Phase II operation, both Wilks' W statistic and Djauhari's F statistic will be used separately in two control charts. These statistics measure the effect of an additional observation on covariance structure. The last problem is to identify the quality characteristics that contributed to an out of control signal.

1.4 Scope of the Study

The scope of study can be divided into 3 aspects.

1. Theoretical aspect

This aspect covers:

- i. Multivariate data ordering in the sense of centre-outward ordering based on Mahalanobis distance and multivariate data concentration in FMCD and MVV algorithms.
- ii. Two new optimal criteria in order to reduce the computational complexity of data concentration process.
- iii. A simulation study to show that the new algorithm produces the same robust Mahalanobis squared distance as FMCD and MVV algorithms.
- iv. Mathematical derivations of the exact distribution of T^2 in Phase I and Wilks' W statistic in Phase II.
- v. A study of the sensitivity analysis of Phase II operation.

2. Computational aspect

From computational point of view, the scope covers:

- i. Simulation experiments to show that proposed method produces the same MCD set compared to FMCD and MVV but with higher computational efficiency.
- ii. Simulation experiments to study the sensitivity analysis of Phase II operation.

3. Practical aspects

Application in real industrial problem to show the advantages of the method developed in this thesis.

1.5 Thesis Organization

The organization of the thesis is as follows. Chapter 1 briefly overviews the monitoring process in multivariate setting and the needs of robust estimates in Phase I operation. The most widely used methods are mentioned and the objective of the

research is defined. The scope of study is presented. The contribution of the research is stated at the end of Chapter 1. Chapter 2 covers the literature review. The existing theory of robust estimation methods and the evolution of ideas in high breakdown point robust estimation methods are presented.

Later on in Chapter 3, critiques to data concentration process in FMCD will be delivered. Furthermore, in Chapter 4, a new robust method with lower computational complexity will be proposed. A new algorithm of robust estimation method is developed. An application of the proposed high breakdown robust estimation method in Phase I of monitoring process variability based on individual observations will be discussed in Chapter 5. The procedure of control charting by using W statistic and F statistic in Phase II will be presented and the relationship between Hotelling's T^2 statistic and W statistic will be showed.

In order to show the performance of both statistics, in Chapter 6 a sensitivity analysis in terms of the percentage of outlier detection and the percentage of false positive and false negative will be presented and discussed. The root causes analysis in order to identify the variables that contribute to an out-of-control signal will be conducted. By using real industrial data, the sensitivity to the change of covariance structure of both W and F control chart will be demonstrated in Chapter 7. Chapter 8 concludes the research results followed by a discussion and recommendations for further improvements.

1.6 Contribution of the study

The contributions of this research can be classified into two parts as follows:

Contribution to the country:

This thesis explains in details a procedure of robust monitoring process variability based on individual observations in multivariate setting. Therefore, we optimistic that

the results and findings from this thesis will be useful for the practitioners in Malaysia manufacturing industries to control and monitor their product and process.

Contribution to the field:

The contribution to the fields of robust statistics and statistical process control can be described into two aspects:

1. Theoretical impact: The novelty of this thesis can be described as follows.
 - i. Since MVV is computationally simpler than FMCD (Wilcox, 2012) and MVV is refinement version of FMCD (Neykov *et al.*, 2012), in this thesis the process of C-step will be refined. Then, a new optimality criterion is developed.
 - ii. Simulation experiments show that the result of the proposed method in terms of running time is far better than FMCD and even better than MVV.
 - iii. Pedagogically, the proof given by Wilks (1962, 1963) for the distribution of W is still difficult to digest. In this thesis, that distribution will be derived by using MANOVA point of view.
 - iv. The relationship between W and T^2 statistics is derived.
 - v. A new test for multivariate normality is introduced.
 - vi. Simulation experiment show that Djauhari's F statistic is more sensitive than Wilks' W statistic to the change of covariance structure in terms of false positive and false negative.
 - vii. A root cause analysis of an out-of-control signal for F chart is proposed. The root causes analysis of W chart can be found in Mason *et al.* (2010).
2. Manufacturing industrial aspect.

A user friendly coding by using Matlab software and Microsoft Excel is developed.

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