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THE IN-CONTROL PERFORMANCE OF THE ROBUST MULTIVARIATE SYNTHETIC CONTROL CHARTS FOR MONITORING MEAN SHIFT

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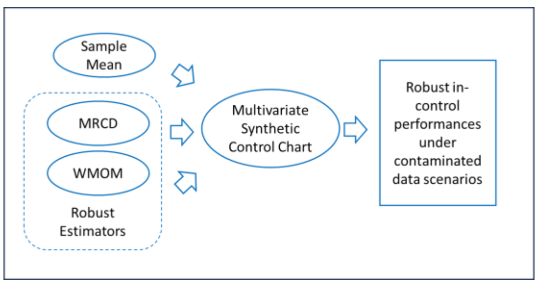
Graphical abstract



Abstract

Multivariate synthetic control chart enables monitoring of multiple process variable simultaneously and hence, negate the inflation of false alarm rates as can be seen in an individual statistical chart. A robust version of the synthetic chart is necessary to mitigate the issue faces by the traditional multivariate synthetic chart, which is unable to produce reliable parameter estimates when Phase I data are contaminated. Therefore, this study proposed three new robust multivariate synthetic control charts (C_{MRCD}, C_{WS} and C_{WP}) which were constructed via minimum regularized covariance determinant (*MRCD*) and winsorized modified one-step *M*-estimator (*WMOM*) for efficient process monitoring. The effectiveness of the proposed robust charts was evaluated in terms of false alarm rates by comparing their in-control performances to the traditional multivariate synthetic chart, C_{mean}, which is based on the sample mean. Via extensive simulation studies, the findings indicate that the proposed robust control charts outperform the traditional chart regardless of the dimensions or the level of contaminations in the dataset. The real data study further validates that the C_{MRCD}, C_{WS} and C_{WP} perform better than the C_{mean}. Specifically, the three robust control charts show significant observations, illustrating better capability in monitoring river water quality when compared to the C_{mean}, i.e., the traditional multivariate synthetic chart.

Keywords: Control Chart, False Alarm Rate, Multivariate Synthetic Control Chart, Robust Estimators, Statistical Process Control

Abstrak

Carta kawalan sintetik multivariat membolehkan pemantauan terhadap pemboleh ubah proses berganda secara serentak dan justeru menafikan kenaikan kadar penggera palsu seperti yang boleh dilihat dalam carta statistik individu. Versi teguh untuk carta sintetik adalah perlu untuk mengendalikan masalah yang dihadapi oleh carta multivariat tradisional, yang mana tidak mampu menghasilkan anggaran parameter yang boleh dipercayai apabila data Fasa 1 tercemar. Oleh yang demikian, kajian ini mencadangkan tiga carta kawalan sintetik multivariate baharu (C_{MRCD}, C_{WS} and C_{WP}) yang dibina menerusi penentu kovarian teratur minimum (*MRCD*) dan penganggar *M*-satu langkah terubah suai terwinsor (*WMOM*) untuk pemantaun process yang cekap. Keberkesanan carta teguh yang dicadangkan dinilai dari segi kadar penggera palsu dengan membandingkan prestasi dalam kawalan carta ini dengan carta sintetik multivariat tradisional, C_{mean}, yang berasaskan kepada min sampel. Menerusi kajian simulasi yang meluas, dapatan menunjukkan bahawa carta kawalan teguh yang dicadangkan mengatasi prestasi carta tradisional tanpa mengira dimensi atau tahap pencemaran di dalam set data. Kajian data sebenar seterusnya mengesahkan bahawa C_{MRCD}, C_{WS} and C_{WP} berprestasi lebih baik daripada C_{mean}. Secara khususnya, tiga carta kawalan teguh ini mempamerkan pemerhatian yang bererti, menggambarkan keupayaan yang lebih baik dalam memantau kualiti air sungai apabila dibandingkan dengan C_{mean}, iaitu carta sintetik multivariat tradisional.

Kata kunci: Carta Kawalan; Kadar Penggera Palsu; Carta Kawalan Sintetik Multivariat; Penganggar teguh; Kawalan Proses Statistik

1.0 INTRODUCTION

To ensure quality of an output, statistical process control (SPC) which comprises real time process monitoring tools that utilize statistical techniques can be applied to monitor and perform necessary control on a process quality characteristic. With the complexity of the processes nowadays, more than one quality characteristics are usually monitored to predict the quality of the outputs. Thus, a multivariate control chat is in need. Utilizing individual control charts for monitoring several related quality characteristics separately can easily inflate the overall false alarm rate in the process [1, 2]. This is mainly due to the interaction between the process quality characteristics that may be overlooked when they are monitored separately [3, 4].

A simple multivariate control chart, Hotelling's T^2 control chart (henceforth denoted by T^2 chart) is effective for a large shift detection that may be caused by a small number of outliers [5]. However, T^2 chart is insensitive to moderate and small shifts in the process [6, 7]. According to Hawkins and Zamba (2003), if small shifts are failed to be detected in a process, a company will incur a larger total cost than a quick detection of large shifts in the long run [8]. To overcome the T^2 chart's limitation, Ghute and Shirke (2008) introduced a multivariate synthetic control chart that integrates the T^2 chart with a conforming run length chart (*CRL*) [9]. This new chart improves the detection across a wider range of shifts [10]. However, like the T^2 chart, this improved multivariate chart still relies on the normality assumption whereby the persistent use of the chart will lead to false signals in non-normally distributed data. To tackle this issue, Khoo *et al.* (2009) proposed a heuristic approach via weighted variance (WV) method [11]. However, this approach only works for skewed distributions since the WV method decomposes a skewed process distribution into two symmetrical distributions. As such, the issue of non-normality such as inflated false alarm rates remain in the case of a symmetrical distribution with heavy tails.

Using robust statistics instead of the sample mean proves to be a superior choice for monitoring changes in non-normal data via the application of control charts [12]. In one of the studies by Abdul-Rahman *et al*. (2021), an application of robust estimators, specifically modified one-step *M*-estimators (*MOM*) and winsorized modified one-step *M*-estimator (*WMOM*) in the univariate synthetic control chart leads to an enhanced robustness of the chart in the context of heavy-tailed distributions upon small process shifts [13]. Therefore, the robustness of the multivariate synthetic control chart can certainly be expected to be improved by the application of robust estimators in reducing the impact of the outliers which are the main cause of non-normality.

In this paper, three new robust control charts were constructed via minimum regularized covariance determinant (*MRCD*) and *WMOM* estimators [14, 15]. Their in-control robustness to the normality assumption was evaluated using the false alarm rate. Their in-control performances were also compared with traditional multivariate synthetic control chart which is based on the sample mean. In the following section, explanations for the chosen location estimators as well as procedures involved in constructing the proposed robust multivariate synthetic charts are given.

2.0 METHODOLOGY

2.1 Descriptions of Robust Estimators

Two robust location measures namely, the *MRCD* and *WMOM*, were applied in the construction of the proposed robust multivariate synthetic control charts. Meanwhile, the sample mean was employed for comparison purposes.

- ***MRCD***: The *MRCD* is a location measure that has been extended from the generalized minimum covariance determinant (*MCD*) to a high dimension by Boudt *et al.* (2020) [14]. Notably, the *MCD* poses the highest possible breakdown point value, i.e., 0.5 [16, 17]. In *MRCD*, the scatter matrix is formed as a convex blend of a target matrix and the sample covariance of the subsets. This estimator is dimension independent, (i.e., able to produce an accurate estimate even when the dimensions exceed the sample size, *n*) while still maintaining the robustness of the *MCD* estimator [14]. Studies by Bulut (2020) and Schreurs *et al.* (2021) affirm the *MRCD*'s effectiveness in outlier detection, even for high-dimensional data, highlighting its value for methodological improvement [18, 19]. The *MRCD* formula is shown below:

$$\hat{\Sigma}_{MRCD} = \underset{H_{\epsilon}\mathcal{H}}{argmin}\left(det\left(\hat{\Sigma}^{H}_{reg}\right)\right)$$

- **WMOM**: The *WMOM* as introduced by Haddad *et al.* (2013), extends the capabilities of its predecessor, *MOM*, to effectively mitigate the effect of outliers [15]. Similar to the *MOM*, the *WMOM* has 50% breakdown point due to the use of the sample median in trimming the outliers, but rather than discarding the outliers, it replaces the supposedly trimmed observations with the highest and lowest values from the remaining data. The *WMOM* formula is shown below:

$$\hat{\theta}_j = \frac{\sum_i^{n_j} X_{i(j)}}{n_j}$$

Where:
$X_{i(j)}$= the i^{th} observations in sample *j* (following the substitution of trimmed values),
n_j = number of observations for sample *j*.

It is noted that:

$$X_{i(j)} = \begin{cases} X_{(i_1+1)j}, if\ (X_{ij} - \hat{M}_j) < -2.24\ (MADn_j) \\ X_{(i)j}, \quad if - 2.24\ (MADn_j) \le (X_{ij} - \hat{M}_j) \le 2.24\ (MADn_j) \\ X_{(n_j - i_2)j}, if\ (X_{ij} - \hat{M}_j) > 2.24\ (MADn_j) \end{cases}$$

Where:
i_1 = number of observations X_{ij} such that $(X_{ij} - \hat{M}_j)$ < -2.24$(MADn_j)$
i_2 = number of observations X_{ij} such that $(X_{ij} - \hat{M}_j)$ > 2.24$(MADn_j)$

Where:
$$MADn = b\ med_i\left|x_i - med_j x_j\right|$$

Typically, *b* is set at 1.4826 to maintain the estimator's consistency under normality

- **Mean**: The sample mean provides the most precise estimation with the smallest standard error in normal distribution scenarios. However, it has a breakdown point of 0 which makes the computation easily affected by outliers. Sample mean formula is shown below:

$$\bar{X} = \frac{\sum_i^n X_i}{n}$$

Two robust location estimation techniques, the *MRCD* and *WMOM*, play a key role in estimating the location vector within the framework of the multivariate synthetic control charting when the process mean is unknown. The *MRCD* generates its own covariance matrices. Meanwhile, in this study, the *WMOM* was paired with:

(i) the product of the percentage bend correlation (ρ_p) and the highly robust scale estimator Q_n; and
(ii) the product of Spearman's rho (ρ_s) and Q_n.

Combining these two location measures with their corresponding covariance matrix estimation methods leads to three newly proposed robust multivariate synthetic control charts. These robust charts and their corresponding estimators are presented in Table 1.

Table 1 The proposed robust control charts with their corresponding estimators

Location Vector	Covariance Matrix	Chart's Notation
MRCD ($\bar{X}_{MRCD}$)	*MRCD* (S_{MRCD})	C_{MRCD}
WMOM ($\bar{X}_W$)	Percentage Bend Correlation x Qn (ρ_p x Qn)	C_{WP}
	Spearman rho x Qn (ρ_s x Qn)	C_{WS}

2.2 Procedures in the Study

The construction of the multivariate synthetic control charts involves two phases namely, Phase I and Phase II. In Phase I, process parameters were estimated using historical data and subsequently, they were used to construct control limits for Phase II process monitoring. Process monitoring in Phase II entails continuous monitoring of prospective samples. Due to challenges in collecting multivariate data in rational subgroups, individual observations were used in Phase II for process monitoring and hence, in evaluating the newly proposed robust control charts.

The structure of the traditional multivariate synthetic control chart combines salient features from the T^2 and *CRL* charts. Notably, the estimation of optimal parameters, *CL* (for T^2 chart) and *L* (for *CRL* chart), were determined in Phase I. Both *CL* and *L* are the control limits of the respective charts whereby their optimal values were generated based on the user-specified false alarm rate and a shift expected to occur in the process.

In this study, the robustification process started by substituting classical location and covariance matrix with their robust counterparts in the T^2 chart. The T^2 statistic is defined as below [20]:

$$T^2 = (X_i - \mu)^T \Sigma^{-1} (X_i - \mu)$$

where *i* = 1,…,n, with i^{th} ordered observations, μ is the mean and Σ^{-1} is inversed matrix of pooled variance-covariance matrix with *p*-dimension. In this study, for each robust multivariate synthetic control chart, the term μ and Σ^{-1} were estimated using robust estimators and the corresponding robust covariance matrix as displayed in Table 1.

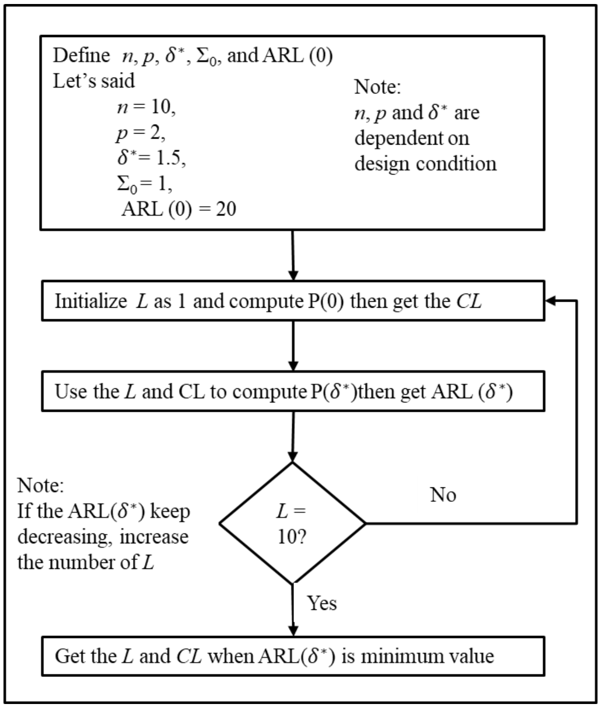
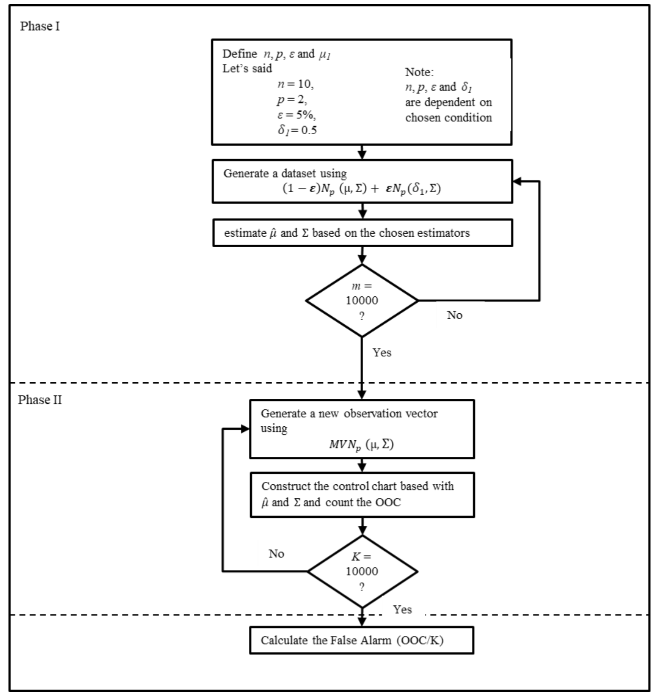


Figure 1 Flowchart to derive optimal parameters for robust control charts



Note: m = number of iterations in Phase I, k = number of Iteration in Phase II, OOC = out of control sample

Figure 2 Flowchart of Phase I & Phase II procedures

The construction of the robust control charts starts with the determination of optimal parameters (i.e., *CL* and *L*) following the process presented in Figure 1. Table 2 lists the optimal values of the *CL* and *L* derived in the study via the R statistical software. Similarly, the iterations involve in Phase I and Phase II procedures as depicted in Figure 2 were generated using the R software.

Table 2 The proposed control charts with their corresponding estimators

		C_{mean}		C_{MRCD}		C_{WS}		C_{WP}	
p	**n**	***CL***	***L***	***CL***	***L***	***CL***	***L***	***CL***	***L***
2	10	5.31	2	27.24	5	6.01	2	7.22	4
	25	4.13	2	7.21	3	4.63	3	4.61	3
	50	4.17	4	6.08	4	3.90	3	3.99	3
	100	3.80	3	4.75	3	3.94	3	4.00	3
	200	3.80	2	5.10	5	3.75	2	3.87	3
	500	3.99	4	4.79	6	4.07	4	4.13	4
10	50	21.09	4	39.68	3	18.96	2	19.73	3
	100	16.81	3	23.09	3	16.39	3	16.82	3
	200	15.27	3	17.99	2	15.07	2	15.54	3
	500	13.83	2	15.50	2	13.84	2	13.98	2
15	100	24.52	2	37.17	2	24.36	2	24.51	2
	200	22.27	2	27.32	2	21.69	2	22.01	2
	500	20.52	2	22.67	2	20.28	2	20.58	2

2.3 Variables Manipulated

Four variables were manipulated to establish different scenarios that include dimensions, i.e., the number of quality characteristics (*p*), the number of sample size (*n*), the proportion of contamination (ε) and the mean shifts (δ_1). Table 3 presented the variable manipulation setting for each of the variables.

Table 3 The variables manipulation in the study

Quality Characteristics (p)	Sample Size (n)	Proportion of Contamination (ε)	Mean Shifts (δ_1)
2	10, 25, 50, 100, 200, 500	10%, 20%	0.25, 1.25, 2, 5
10	50, 100, 200, 500	10%, 20%	0.25, 1.25, 2, 5
15	100, 200, 500	10%, 20%	0.25, 1.25, 2, 5

As the aim of this study is to compare the in-control performances between the newly proposed robust charts and the traditional multivariate synthetic chart, the pairing of *p* and *n* is restricted to values that satisfy $n > 5p$. This is to ensure that the estimation of the covariance matrix can be executed for all charts under investigation. Thus, avoiding the singularity issue.

3.0 RESULTS AND DISCUSSION

To assess the robustness of the proposed multivariate synthetic control charts under an in-control condition, Bradley's stringent criterion of robustness was applied where a chart is deemed robust if it can maintain the false alarm rate (FAR) within this range of interval: $0.9\alpha \leq \hat{\alpha} \leq 1.1\alpha$ where α is the user-specified FAR. In this study, α is set at 0.05 and thus, a chart is considered robust if it can yield a value of FAR within this interval: [0.045, 0.055].

3.1 Simulation Study Analysis

The simulation results shows that the three newly proposed robust multivariate synthetic control charts, i.e., C_{MRCD}, C_{WS} and C_{WP}, perform better than the traditional chart, C_{mean}, across the majority of the simulation's scenario. In the bivariate case, i.e., when p = 2, the proposed robust control charts overtake the traditional control chart's performance when the mean shift, δ_1, is large. The difference of the FAR values for the C_{mean} when compared to the Bradley's stringent criterion is getting larger when the value of δ_1 increases. This is observed for all n. Meanwhile, the C_{MRCD}, C_{WS} and C_{WP} yield the FAR values close to Bradley's stringent criteria. Comparing the three newly proposed robust control charts, the C_{MRCD} is the best in controlling the FAR. Unlike other charts observed in the study, the C_{MRCD} does not deviate much from the Bradley's stringent robust criteria when the value of δ_1 increases. This is true for all n, especially when ε = 10%, as shown in Figures 3 – 4 (focusing on the graphs for p = 2).

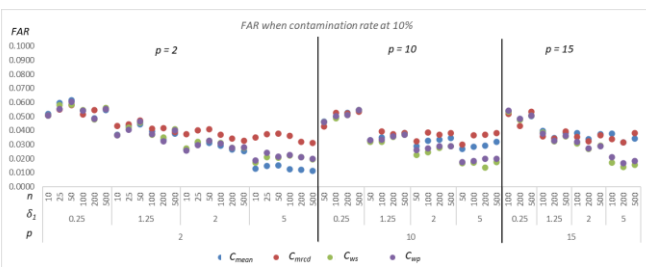


Figure 3 FAR when contamination rate at 10%

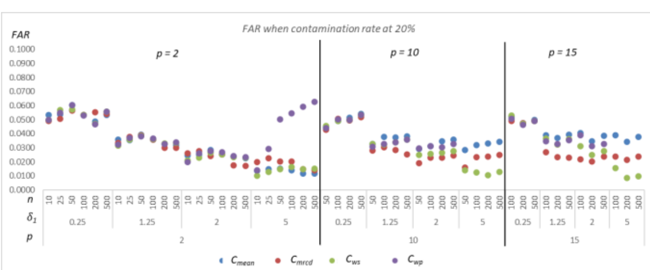


Figure 4 FAR when contamination rate at 20%

At the same level of contamination, i.e., ε = 10%, when p increases, the C_{MRCD} continues to outperform the C_{mean}, as illustrated in Figure 3 (focusing on the graph for p =10). It is evident that the FAR values for the C_{MRCD} have a smaller gap to the Bradley's stringent robust criteria when compared to the rest of the charts. However, the C_{MRCD} does not perform as expected when the proportion of the contamination, ε, is getting larger as shown in Figure 4, for p =10. Under this scenario, the C_{mean} is yielding the FAR values closest to the robust interval.

For p =15 and ε = 10%, the C_{MRCD} and C_{mean} perform comparably. Yet, upon dire contamination (ε = 20%), the FAR differences between the robust chart and the traditional chart are quite significant whereby the C_{MRCD} yields the FAR value that slightly deviate from the Bradley's stringent robust criteria.

3.2 Real Data Application

In this study, the proposed robust control charts were also applied on water quality data retrieved from http://smg.asma.com.my:98/. The system focuses on monitoring the river water quality at Kampung Medan, Selangor. Five water quality characteristics were identified which include chemical oxygen demand (COD), ammoniacal nitrogen (NH3N), potential of Hydrogen (pH), dissolve oxygen (DO) and total suspended solids (TSS). In general, water quality can be categorized into five levels which are Class I to Class IV. The river water quality is considered polluted when a measurement falls in Class II to Class IV whereas higher classes imply severe pollution scenarios. In our case, the water quality at Kampung Medan is at Class III for most of the measurements recorded. In applying the proposed control chart to the data, measurements that had been categorized as Class IV and Class V will be considered as out-of-control. A good chart would be able to flag the Class IV and Class V measurements as out-of-control observations while the Class III measurements are considered as in-control observations which represent the common river water quality in Kampung Medan.

Out of 428 data collected, 300 of them were used in Phase I for the location vectors and covariance matrix estimation. The remaining 128 data were used in Phase II for monitoring the river quality.

Tables 4a to 4d present the confusion matrix for the C_{mean}, C_{mrcd}, C_{wp} and C_{ws} under real data study. The header row represents the true river water quality in Kampung Medan in which Class IV represents an out-of-control situation and Class III represents an in-controls water state. The header column represents the results flagged by the multivariate synthetic control charts in this study.

The green-colored cells represent the number of observations that are match with the real data. Those out-of-control cases in the real data are flagged as an out-of-control situation by the control charts and likewise, for the in-control cases. Meanwhile, the orange-colored cells show a false flagged by the control charts.

As presented in Tables 4a to 4d, the proposed robust multivariate synthetic control charts, i.e., C_{mrcd}, C_{wp} and C_{ws}, can identify all 107 Class III's river water quality as in-control, while C_{mean} is only able to identify

99 of them. On the other hand, for the Class IV's river water quality, the three proposed robust control charts were only able to identify 17 out of 21 cases, as opposed to 19 by C_{mean}. For a more extensive assessment, we summarize the performance of the charts based on specificity and predictive values as depicted in Table 5.

Table 4a Confusion matrix of the C_{mean} on real data application

		Real Data		
		Out of Control (Class IV)	**In Control (Class III)**	
C_{mean} Trigger	**Out of Control**	19	8	PPV =70 %
	In Control	2	99	NPV = 98%
		Sensitivity = 90%	Specificity = 93%	

Table 4b Confusion matrix of the C_{mrcd} on real data application

		Real Data		
		Out of Control (Class IV)	**In Control (Class III)**	
C_{mrcd} Trigger	**Out of Control**	17	0	PPV =100 %
	In Control	4	107	NPV = 96%
		Sensitivity = 81%	Specificity = 100%	

Table 4c Confusion matrix of the C_{wp} on real data application

		Real Data		
		Out of Control (Class IV)	**In Control (Class III)**	
C_{wp} Trigger	**Out of Control**	17	0	PPV =100 %
	In Control	4	107	NPV = 96%
		Sensitivity = 81%	Specificity = 100%	

Table 4d Confusion matrix of the C_{ws} on real data application

		Real Data		
		Out of Control (Class IV)	**In Control (Class III)**	
C_{ws} Trigger	**Out of Control**	17	0	PPV =100 %
	In Control	4	107	NPV = 96%
		Sensitivity = 81%	Specificity = 100%	

Note:
Sensitivity = The ability of detect out-of-control water quality scenarios
PPV = The detection rate of true out-of-control water quality scenarios
Specificity = The ability of detect in-control water quality scenarios
NPV = The detection rate of true in-control water quality scenarios

In this study, it is anticipated that the proposed control chart can effectively identify an out-of-control scenario which is the measurements of water quality in Class IV. Thus, this is considered as a positive flag when the control chart shows the ability to flag the out-of-control scenarios. Meanwhile, the ability to flag the in-control scenarios is considered as a negative flag. The positive and negative flagging are targeted to assess the performance of the charts; whether they can fittingly detect the river water quality.

In terms of the sensitivity and positive predictive value (PPV), the C_{mean} illustrates that it has a high sensitivity value (90%), which is the ability to identify the out-of-control cases. The percentage is higher than demonstrated by the three robust control charts. The sensitivity values of the C_{mrcd}, C_{wp} and C_{ws}, are slightly lower (81%). However, the PPV of the robust control charts is higher, which is 100%, when compared to the C_{mean}, which is only at 70%. In terms of the specificity and negative predictive value (NPV), the C_{mrcd}, C_{wp} and C_{ws} have a balance performance, that is, the specificity and NPV are at 100% and 96%, respectively. Conversely, the C_{mean} has specificity and NPV of 93% and 98%, respectively. This shows that the C_{mrcd}, C_{wp} and C_{ws} are able to predict the Class III river water quality fittingly.

Table 5 Sensitivity, specificity, and predictive values for real data applications

Control Charts	Sensitivity	PPV	Specificity	NPV
C_{mean}	90%	70%	93%	98%
C_{mrcd}	81%	100%	100%	96%
C_{wp}	81%	100%	100%	96%
C_{ws}	81%	100%	100%	96%

4.0 CONCLUSION

In the simulation study, it can be observed that the in-control performances of the robust multivariate synthetic control charts namely, C_{mrcd}, C_{wp} and C_{ws}, surpass the traditional multivariate synthetic chart, i.e., C_{mean}. The assessment based on the false alarm rate (FAR) was conducted via extensive simulation studies by manipulating variables such dimensions, sample size, contamination level and shift size. In particular, the robust C_{mrcd} chart exhibits the most stable in-control performance, when compared to the others control chart in this study. Regarding the real data application, the three newly proposed robust control charts demonstrate equal capability in detecting both out-of-control and on-control river water quality. Thus, validating the strengths of the performance of the proposed robust charts as demonstrated in the simulation studies. In future, it is recommended to further investigate the out-of-control performance of the three proposed robust multivariate synthetic charts by extending the scenarios to cover high-dimensional data.

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Conflicts of Interest

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper.

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