Monitoring Nonlinear Profiles Using Wavelets

M. Nikoo, R. Noorossana

M. Nikoo, Department of Industrial Engineering, Science and Research Branch, Islamic Azad University, Tehran,Iran
R. Noorossana, Department of Industrial Engineering, Iran University of Science and Technology, Tehran, Iran

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ABSTRACT

In many manufacturing processes, the quality of a product is characterized by a non-linear relationship between a dependent variable and one or more independent variables. Using nonlinear regression for monitoring nonlinear profiles have been proposed in the literature of profile monitoring which is faced with two problems; 1) the distribution of regression coefficients in small samples is unknown and 2) with the increasing complexity of process, regression parameters will increase and thereby the efficiency of control charts decreases. In this paper, wavelet transform is used in Phase II for monitoring nonlinear profiles. In wavelets transform, two parameters specify the smoothing level, the first one is threshold and the second one is decomposition level of regression function form. First, using the adjusted coefficient of determination, decomposition level is specified and then process performance is monitored using the mean of wavelet coefficients and profile variance. The efficiency of the proposed control charts based on the average run length (ARL) criterion for real data is compared with the existing control charts for monitoring nonlinear profiles in Phase II

1. Introduction

In many production processes, quality of a product can be defined using the relationship between a dependent variable and one or more independent variables. This relationship is defined as profile. In practical applications, profiles are observed as linear (simple and multiple), polynomial, and nonlinear forms. Monitoring profiles is studied in Phases I and II. Phase I aims at determining the stability of the process and estimating the unknown parameters of the process whereas Phase II aims at identifying the changes in process parameters. In recent years, several methods are presented for monitoring different types of profiles by researchers in Phases I and II. Kang and Albin [1] proposed a multivariate T^2 control chart for monitoring regression parameters and EWMA / R chart for monitoring mean and variance in simple linear profiles in Phase II. After coding independent variable, Kim et al. [2] separated regression parameters from each other and used three independent EWMA control charts to monitor intercept, slope, and variance separately. Mahmoud and Woodal [3] used regression based on dummy variables for monitoring process mean by integrating

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Corresponding author: *R. Noorossana*
Email: rassoul@iust.ac.ir

observations from all samples and used a F statistic to monitor variance. Noorossana et al. [4] proposed procedures for the case of correlation between error terms. Some methods were also presented for monitoring multiple linear profiles, polynomial profiles, and simple and multivariate profiles in Phases I and II by Mahmoud [5], Kazemzadeh et al. [6], and *Noorossana* et al. [7].

Walker and Wright [8] and Williams et al. [9] presented real examples of non-linear relationships between the dependent variable and independent variable. Williams et al. [9] proposed the use of T^2 control chart based on parameters estimated by nonlinear regression in Phase I. They compared the performance of multivariate T^2 control chart based on three methods of estimating the variance – covariance matrix. Jensen and Breech [10] proposed using nonlinear mixed models for monitoring nonlinear profiles in the case of correlation between residual within profiles. Vaghefi et al. [11] developed parametric and nonparametric methods for monitoring linear profiles in Phase II.

Control charts based on nonlinear regression parameters faces two problems. First, the distribution of regression parameters in small samples (even in case of normal observations) is not known. Second, with the increasing complexity of the process and its non-stationary behavior, one needs many regression parameters which will reduce power of the test used for monitoring multivariate structure of the observations. Due to these shortcomings of non-linear regression in monitoring nonlinear profiles, many researchers have used nonparametric regression to model and estimate the parameters. In parametric regression (linear and nonlinear) regression function form is pre-defined. And the goal is to estimate the regression function with the least number of parameters. In other words, one parameter (one variable) is added to the model only when it leads to the reduction of mean square error. In nonparametric regression or smoothing, the regression function form is not predetermined and it is selected based on the intended use which provides the desirable

level of smoothing. Hence, what makes the difference between the two approaches is that in nonparametric regression, the goal is not to estimate the model with minimum number of parameters. Some known functions with certain properties such as differentiability are used as the bases function which among them one can name Fourier, Splines, Wavelets, and Kernel function. Given the capabilities of wavelet basis functions for modeling non-stationary processes with sharp changes, several researchers used discrete wavelet transform and (nonparametric regression) in monitoring non-linear profiles. Jen and Shi [12] reduced the profile dimensions using the concept of universal threshold and proposed applying multivariate T^2 statistic based on significant wavelet coefficients for monitoring purposes in Phase II. Lada et al. [13] used minimizing Akaike Information Criterion (AIC) to determine the decomposition level of wavelet coefficients.

Jeong and Lu [14] considered the inefficiency of parametric regression in detecting local shifts and proposed a new threshold that is updated for each profile in Phase II and evaluated the effectiveness of the designed control chart (based on wavelet coefficients greater than this threshold) using average run length criterion. Zou et al. [15] used the combination of Haar wavelet and statistical process control to monitor waveform signals. They proposed the use of a control chart for each wavelet coefficient using Bonferroni control limits. Chicken et al. [16] proposed the use of a semi-parametric regression based on wavelet functions to detect changes in a sequence of profiles. Paynaber and Jin [17] used random effects models with wavelet transform to monitor within and between profiles shifts simultaneously. Two important issues faced when using wavelet transform for smoothing purposes are compression level and de-noising. De-noising is used to get rid of random errors from observations whereas compression refers to dimension reduction of the data in such a way that the original information about profile is remained unchanged. Determining the threshold parameters and decomposition level (scale)

specifies the regression function. By increasing the decomposition level, the number of parameters used in approximation (estimation) of curve and subsequently the goodness of fit is reduced. In other words, the decomposition level determines the regression function form and thus specifies the number of parameters that can affect the power of T^2 statistic test. So it is necessary to select the level of decomposition so that with minimum number of coefficients the curve with similar shape is obtained. In this paper, to monitor variability in average profile, a multivariate T^2-statistic based on scale functions coefficients of the wavelet will be used and to monitor variability within the profile a control chart based on wavelet coefficients will be used. To describe the method for selecting scale and to compare the effectiveness of the proposed control charts for monitoring mean and variance, the vertical density profile (VDP) of Walker and Wright [8] is used.

Next section discusses the discrete wavelet transform, the thresholds, and the smoothing parameters of wavelet analysis and variance estimators. The third section explains how the decomposition level is determined. Section four describes statistics for monitoring variability within profile and monitoring variability in the process mean. In the fifth section, the current methods for monitoring non-linear profiles in Phase II are presented. Using VDP data, the performance of the proposed control charts for monitoring the mean and variance are compared with the existing methods discussed in section four. In Section seven, conclusions and recommendations for further research in the nonlinear monitoring profiles using wavelet transform are presented.

2. Wavelet Transform

Wavelets are a family of basis functions which enjoy more capability of modeling the functions with complex behavior and sharp changes to the basis functions such as Furrier and Splines. The main element of the wavelet structures are scale functions $\phi(x)$ defined as

$$\phi_{jk} = 2^{\frac{j}{2}} \phi\left(2^j x - k\right) \tag{1}$$

Equation (1) is the translated version of k and dilated (change of scale) version of j in the $\phi(x)$ function. Function $\psi_{jk} = 2^{\frac{j}{2}} \psi\left(2^j x - k\right)$ is built based on function ϕ_{jk}. If $f(t) \in L^2$ then $f(t)$ can be written as following using basis functions of wavelet [18]:

$$y = \sum_{k=0}^{2^{j_0}-1} c_{j_0 k} \phi_{j_0 k} + \sum_{j=j_0}^{J-1} \sum_{k=1}^{2^J-1} d_{jk} \psi_{jk} \qquad c_{j_0,k} \tag{2}$$

coefficient shows low frequency variations (macro-scale variations) and $d_{j,k}$ is high frequency variations (micro-scale variations). One of the most important features of wavelets transform is the possibility of dilation of functions with scale variation (j_0). J_0 is the analysis level in wavelets transform and full analysis (smallest scale) according to Equation (3) is determined using pyramid algorithm:

$$n = 2^j \tag{3}$$

2-1.   Dimension Reduction in the Wavelets Transforms

Every observation of y_i in the profile is formed of a non-random component $f(x_i)$ and a random component of ε_i as $y_i = f(x_i) + \varepsilon_i$. It is assumed that the random component has normal distribution and is independently and identically distributed (iid). To reduce the data size, the compression concept and de-noising are used. The objective of compression is dimension reduction in such a way that that the main information regarding the curve is lost.

In de-noising, our objective is detecting the main signal from the observations with noise. Therefore, that set of wavelet coefficients that model the small changes (most often $d_{j,k}$ coefficient) are put aside from the model. In compression and de-noising steps, setting thresholds such that coefficients smaller than

the threshold can be deleted is a significant point in reducing data dimension. In both methods, threshold acts on $d_{j,k}$ coefficients in Equation (2) $(j \ge j_0)$ and has no effect on $c_{j_0,K}$.

Therefore, before applying the threshold on wavelet transform coefficients, proper scale should be selected from numbers $j = 0,1,2,3,...,J-1$ in Equation (2). For different scales and thresholds, the number of coefficients deleted would be different. Two methods of hard threshold function and soft threshold function are defined for applying threshold on wavelet transform coefficients. In the literature, various thresholds are introduced for size reduction.

$$\lambda = \hat{\sigma}\sqrt{2\log n} \qquad (4)$$

Equation (4), due to interesting features and simplicity is the most frequently used threshold in the wavelet literature and is called universal threshold. Since this threshold leads to the reduction of MSE with increasing number of data points in each curve, it is commonly used in nonparametric regression.

2-2. Estimation of Variance in Nonparametric Regression Using Wavelets

In parametric regression (linear, polynomial, and nonlinear), the ratio of mean square error of the residual regressions to degrees of freedom $(\hat{\sigma}^2 = \dfrac{\sum_{i=1}^{n} e_i^2}{n-k})$, is used as variance estimator. In nonparametric regression, using wavelet basis functions for estimation of standard deviation and variance of observations, two estimators of given in Equations (5) and (6) are introduced [19]. Equation (5) is the estimator for median of the absolute deviation (MAD). Estimator of the standard deviation in Equation (5) is a robust estimator with respect to scale.

$$\hat{\sigma} = \frac{median\left|d_{J-1,k}\right|}{.6745} \qquad (5)$$

$$\hat{\sigma}^2 = \frac{\sum_{k=1}^{n/2}(d_{J-1,k}-\overline{d}_{J-1})^2}{(\frac{n}{2}-1)} \qquad (6)$$

3. Determining Decomposition Level in DWT

According to pyramid algorithm, in the j the scale and using Equation (2), data are mapped to two sets c_{jk} and d_{jk} where the number of coefficients indicate the signal at level j (c_{jk}) would be half of level j+1. Accordingly, with the increase of scale (reduction of j), the number of coefficients which define signal would reduce noticeably. One of the common criteria for determining the goodness of fit in regression analysis is the coefficient of determination. Coefficient of determination (R^2) is a criterion that shows how good the regression function is fit to a set of data points. Total sum of squares (TSS) associated with total variation around the mean of the dependent variable can be divided to as sum of squares due to estimated sum of squares (ESS) and residual sum of squares (RSS) or

$$\left[\sum_{i=1}^{n}(y_i - \overline{y})^2 = \sum_{i=1}^{n}(\hat{y}_i - \overline{y})^2 + \sum_{i=1}^{n}(y_i - \hat{y}_i)^2\right] \quad (7)$$

Coefficient of determination in bivariate regression (R^2) is obtained by dividing ESS by TSS. Coefficient of determination does not decrease by increasing the number of ESS. Thus, adjusted coefficient of determination in Equation (8) will be used for comparing the goodness of fit of regression function with different number of independent variables.

$$\overline{R}^2 = 1 - \frac{(n-1)}{n-k}(1-R^2) \qquad (8)$$

In Equation (8), n is the number of observations and k is the number of parameters (variables number and intercept). Number of scale functions and thereby the number of $c_{j_0 k}$ coefficients will decrease with an increase in the decomposition level. Therefore, we are faced with different number of independent variables for different decomposition level and as mentioned above,

Equation (8) is used for evaluating the goodness of fit of the regression function.

4. Monitoring Nonlinear Profiles Using Wavelets Transform

For DWT data, if observations have normal distribution then wavelet coefficients ($w_{j,k}$) will have an asymptotic normal distribution as n increases [19]. If θj is population parameter (wavelet coefficients) then

$$\sqrt{n}\left(w_{jk} - \theta_{jk}\right) \overset{\text{asy}}{\approx} N(0, \sigma^2) \qquad (9)$$

4-1. Monitoring Average Profile in Global Shift

Using Equation (9), one can use control charts for monitoring a linear profile (simple, multiple and polynomial) in Phases I and II (e.g., T^2, slrt، χ^2, MCUSUM, and MEWMA) to monitor c_{j0k} coefficients. In this paper the following statistics are use:

$$T_l^2 = (Z_l - \bar{Z})' \sum{}^{-1} (Z_l - \bar{Z}) \qquad (10)$$

$$Z_l = \lfloor c_{jkl} \rfloor \qquad k = 0, 1, \ldots 2^j - 1 \qquad (11)$$

In Equation (10), T_l^2 is the statistic for monitoring them mean, Z_l is the $k \times 1$ vector of the wavelet approximation coefficient of the lth profile and $\bar{Z}$ is the average vector for the parameters of wavelet approximation coefficients. In Equation (11), j is the decomposition level of scale. Based on the calculation method for matrix $\sum$, different T_l^2 statistics could be obtained. Sample covariance matrix defined by Equation (12) is used in the multivariate T^2-statistic.

$$\sum = \frac{1}{m-1} \sum_{p=1}^{m} (c_{jp} - \bar{c}_j)(c_{jp} - \bar{c}_j)' \qquad (12)$$

In Equation (12), m is the number of profiles, c_{jp} and $\bar{c}_j$ are vectors of wavelet transform coefficients for the pth profile and the estimation of population parameters, respectively.

4-2. Monitoring Variance within the Profile

Statistic in Equation (6) is used for estimation of standard deviation. Equation (6) presents an estimate of standard deviation within observations (error term) according to standard deviation of wavelet transform coefficients ($d_{J-1,K}$) at the lowest decomposition level with the smallest scale in multi-resolution analysis or first analysis level.

According to Equation (9), if the observations are normal, d_{jk} coefficients obtained in Phase I from in-control profiles are normal too. Therefore, differences of σ_l^2 (variance estimation of l-th profile) are related to random factors and unbiased estimate of the common variance is obtained using pooled data of m profiles (d_{jk} coefficients).

$$\hat{\sigma}^2 = \frac{\sum_{l=1}^{m} \sum_{k=1}^{\frac{n}{2}} \left(d_{ljk} - \bar{d}_{lj}\right)^2}{N - m} \qquad (13)$$

In Equation (13), m is the number of profiles under control, j is the decomposition scale, index k indicates wavelet transform coefficient, and n is the number of profile observations and $N = m\left(\frac{n}{2}\right)$

$$\chi_l^2 = \sum_{k=1}^{\frac{n}{2}} \left(\frac{d_{l,J-1,k} - \bar{d}_{J-1,k}}{\sigma}\right)^2 \qquad (14)$$

In Equation (14), χ_l^2 is the statistic for monitoring variability in the lth profile, $d_{l,J-1,k}$ is the kth wavelet coefficient in the lowest decomposition level for the lth profile and σ is the estimate for observations variance within profile according to Equation (13). χ_l^2 has chi square distribution with $(\frac{n}{2} - 1)$ degrees of freedom.

5. The Existing Methods of Monitoring Non-linear Profiles in Phase II

According to the literature, monitoring nonlinear profiles can be divided into two groups. One group consists of control charts based on nonlinear regression coefficients and in the other group consists of nonparametric

regression coefficients which are used to monitor process mean. Despite widespread use of non-linear profiles in the industry, few papers have studied non-linear profiles. In monitoring nonlinear profiles using regression in Phase I, Williams et al. [9] and in Phase II Vaghefi et al. [11] presented methods for monitoring nonlinear profiles. Since the purpose of this paper is to monitor non-linear profile in Phase II, the results of the proposed methods are compared to results reported by Vaghefi et al. [11]. In the following section, the existing methods for monitoring non-linear profiles using nonlinear regression in Phase II are presented

5-1. Multivariate T2 Control Chart

The multivariate T2 control chart is based on the estimates of regression coefficients (β) and variance - covariance (Σ) matrix obtained in Phase I. The above statistic for the ith profile is calculated using the following equation:

$$T_i^2 = \left(\hat{\beta}_i - \overline{\beta}\right)' \Sigma^{-1} \left(\hat{\beta}_i - \overline{\beta}\right) \quad (15)$$

If P is the number of nonlinear regression parameters, multivariate T^2 control chart has the level of confidence $UCL = \chi_{P,\alpha}^{2}$

5-2. Combination of MCUSUM and X^2

In this method, multivariate cumulative (MCUSUM) control chart is used according to Equation (16) for monitoring the average.

$$S_i = \max(S_{i-1} + a'\hat{\beta}_i - .5D, 0) \quad (16)$$

In this relationship

$$S_0 = 0 \; \text{,} \; a' = \frac{(\beta_\delta - \beta_0)\Sigma_\beta^{-1}}{\sqrt{(\beta_\delta - \beta)'\Sigma^{-1}(\beta_\delta - \beta)}} \; \text{,}$$

$$D = \sqrt{(\beta_\delta - \beta_0)'\Sigma_\beta^{-1}(\beta_\delta - \beta_0)} \; \text{و} \; \beta_\delta = \beta_0 + \delta$$

$$\chi_i^2 = \sum_{j=1}^{n} \left(\frac{e_{ij}}{\sigma}\right)^2 \quad (17)$$

Statistic (17) is a univariate statistic. It's possible to select threshold H according to univariate CUSUM method in such a way to

obtain the desired type I error. To monitor the variance, statistic (17) is used.
In the above relationship, $e_{ij} = y_{ij} - f(x_{ij} - \beta)$ is the difference between the observed profile and the basis profile. The control parameter limit of the Equation (17) is $UCL = \chi_{n,1-\alpha}^{2}$.

6. A Numerical Example

To provide the methods presented in the third and fourth sections, VDP data is used. Vertical density of particles indicates a quality that is monitored at various locations. In the production process, it is specified that thickness in the center of particle panels is below the upper and lower parts. There are 24 profiles and in each profile 314 observations from the vertical density of the board is taken with 002 inches apart (Figure 1).
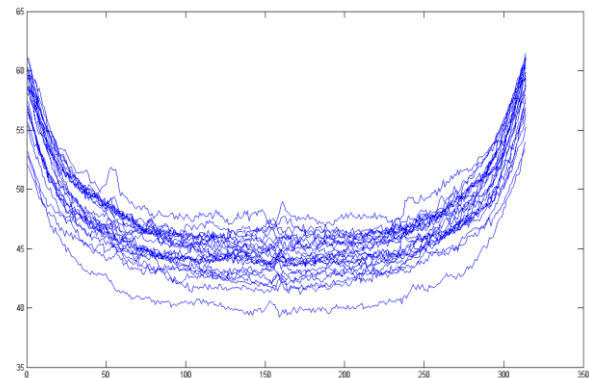

Fig.1. Data of 24 profiles

The number of scales for 314 observations is defined based on Equation (3) is equal to $J = 8$. Therefore, the distance of scale functions at intervals $\left[\frac{k}{2^j}, \frac{k+1}{2^j}\right)$ is defined with j taking values in the range of $j = 0, ..., 7$. In Figures 2, 3, and 4 estimates of VDP data using Haar basis functions is shown for every $j = 2$, $j = 4$ and $j = 6$.
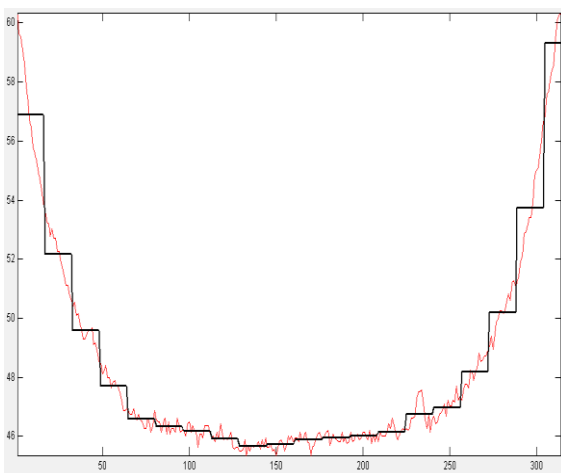By reducing J the number of wavelet coefficients of the regression function is reduced and estimation accuracy is reduced as well. Therefore, choosing the analysis level with the lowest wavelet coefficients and a low frequency ($C_{j0\,k}$) in which the main features of profile is to be included would be of interest.
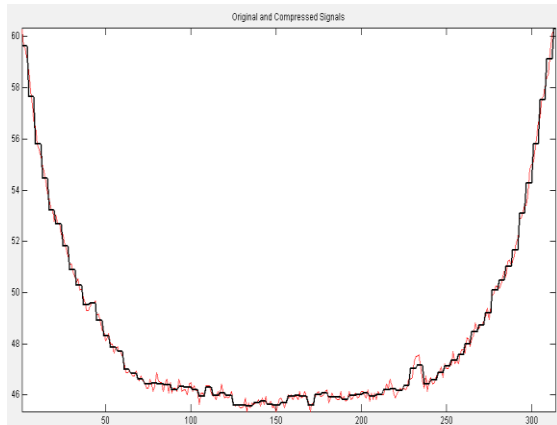
Fig. 2. Estimation by the use of Haar function at Level 2, $j = 6$
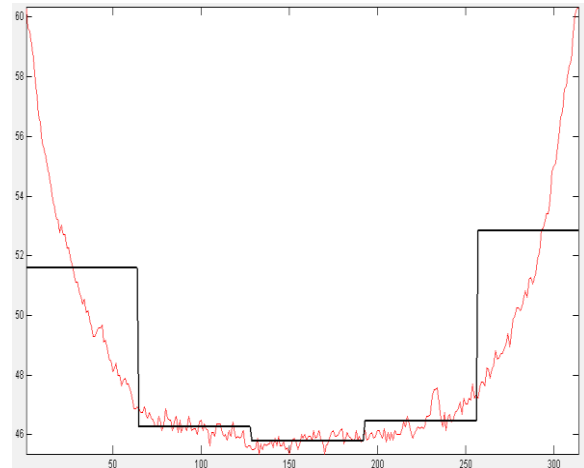
Fig.4. Estimation by the use of Haar function at Level 6, $j = 2$

6-1.   Determining the Decomposition Level

In Table 1, the adjusted coefficients of determination R^2, the number of coefficients and residual sum of square (RSS) is presented at each level of analysis.

Fig.3. Estimation by the use of Haar function in Level 4, $j = 4$

Tab. 1.Adjusted coefficient of determination in different decomposition level

Decomposition level	Number of coefficient	RSS	Coefficient of determination
1	157	6.59	0.998
2	79	19.37	0.995
3	40	56.64	0.986
4	20	167.23	0.96
5	10	578.41	0.86
6	5	1755	0.68
7	3	2678	0.35
8	2	3174	0.23

Coefficient of determination of explanatory percentage of regression function is from the entire observations variation that does not have deflection up to the fourth level of analysis. Therefore, level 4 is selected as the level of analysis and at this level with the help of 20 coefficients instead of 314 observations, only 4% of the data are deleted.

6-2. Comparing the Efficiency of the

Proposed Methods with the Existing Methods
In monitoring VDP data profile, using the method presented in Section III, the best scale of analysis is Level 4. Regression function (Equation 2) with 20 C_{JK} coefficients explained 96% of variation using the dependent variable (Table 1). To monitor the variance of the error term, the proposed method in Section 4 is used based on the statistic given by Equation (14) and to monitor stability in the average of the profiles a multivariate T^2 statistic is used and the combination of these two statistics for monitoring of average and variance of (within the) profile is showed by $T^2 \chi^2$.

The effectiveness of the proposed method is evaluated through a comparison of the results reported by Vaghefi et al. [11] which was presented for the purpose of monitoring non-linear profiles in Phase II. In this method, the combination T^2 and χ^2 defined by Equations (15) and (17) (which are $T^2 \chi^2$ regression) are used for monitoring average and variance.

Nonlinear function presented by Williams et al. [9] for modeling nonlinear bathtub profile is given by

$$f(x_{ij}, \beta) = \begin{cases} a_1(x_{ij} - d)^{b_1} + c & x_{ij} \geq d \\ a_2(-x_{ij} + d)^{b_2} + c & x_{ij} < d \end{cases} \quad (18)$$

In this equation $\beta = (a_1, a_2, b_1, b_2, c, d)$ are the regression parameters estimated using nonlinear regression.

According to Williams et al. [9], profiles No. 15 and 18 that were out of control in Phase I are removed from the model parameters estimation calculations (average and variance) in Equations (10), (13), and (17). Two control charts are designed in a way that in-control *ARL* 200 or $\alpha_{overall}$=0.005. For each monitoring statistic, average and variance the probability of false alarm is obtained according to $\alpha = 1-(1-\alpha_{overall})^{0.5}$ the in-control ARL for the charts would 400. To achieve in-control ARL of 200 for $T^2 \chi^2$–*Regression* control chart, UCL for T^2 and χ^2 are considered as 149.85 and 5.66, respectively.

Also for $T^2 \chi^2$- *Wavelet* control chart, the upper control limits of 210.5 and 42.44 were used for T^2 and χ^2, respectively to achieve overall ARL equal to 200.
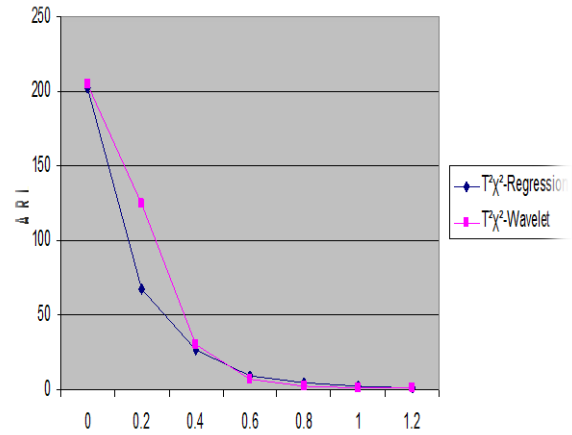

Fig.5. ARL performance under shift in

process average (from *b* to *b+λσ*)
ARL is calculated based on 10000 simulation runs. As you could see, under different shifts in the process average process, $T^2 \chi^2_{\_Regression}$ enjoys better performance compared to the proposed control of the paper $T^2 \chi^2_{-Wavelet}$ (Figure 5). Higher performance of $T^2 \chi^2_{\_Regression}$ is due to lower number of parameters (6 variables) of T^2 statistic compared to T^2 statistic in $T^2 \chi^2_{-Wavelet}$. As the complexity of the functional form of profile increases, it is expected that the performance (effectiveness) of $T^2 \chi^2_{-Regression}$ to be increased to converge to $T^2 \chi^2_{-wavelet}$ control chart.

In monitoring the variability within the profile (the variance of the error term), the performance of the proposed control chart or $T^2 \chi^2_{-wavelet}$ will become better than $T^2 \chi^2_{-Regression}$ control chart (see Figure 6).
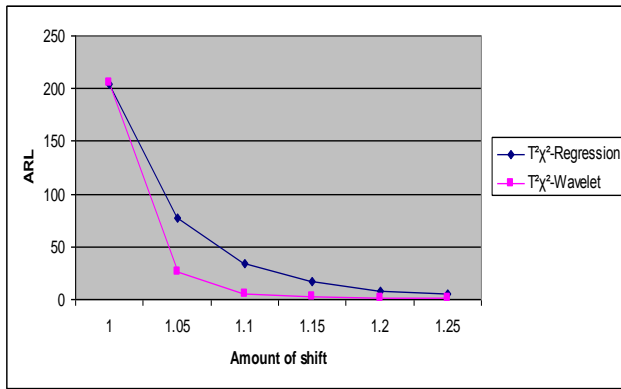
Fig.6. Comparison of control charts under different shift in the process variance (σ to $\lambda\sigma$)

7. Conclusions

The quality of many products can be monitored using a nonlinear relationship between a dependent variable (qualitative properties) and one or more independent variables. Nonlinear regression-based methods for monitoring parameters of these processes have two main problems. First, the distribution of the regression parameters is unknown in small samples and the increasing complexity of the process. Wavelets transform is a powerful method for modeling complex processes and sharp changes that were considered here. In this paper, based on the adjusted coefficient of determination ($\bar{R}^2$) the appropriate decomposition level for wavelets transform is specified and then using the specified decomposition level process average is monitored using a T^2 control chart. Using variance estimators of parametric regression in nonparametric regression provides biased estimates of the variance of the error term. To estimate the variance of error term, the proposed statistics in nonparametric regression literature with wavelets were used and according to that the control chart is presented. The performance of the proposed control charts under a general shift in the mean and variance have been compared to the available control charts based on nonlinear regression using VDP data. Since VDP data does not have many sharp changes, performance of control charts based on nonlinear regression especially in the detection of changes in the process average

outperforms the control chart proposed in this paper. However, as the complexity of the functional form increases, the performance of the proposed chart improves.

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