International Journal of Mathematics and Statistics Invention (IJMSI)
E-ISSN: 2321 – 4767 P-ISSN: 2321 - 4759
www.ijmsi.org Volume 7 Issue 2 || February, 2019 || PP-18-25

A Proposed Spline Smoothing Estimation Method for Time Series Observations

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ABSTRACT*:In this paper, three existing methods used to estimate the degree of smoothness of a Spline Smoothing techniques was compared with a proposed smoothing method for a time series data under the assumption that the error terms are independent. The intention is to investigate the method that is most effective and consistent in estimating smoothing parameters, a simulation program written in R provides a comparison for GCV, GML, UBR and the proposed method, based on sample 20, 60 and 100, for four smoothing parameters 1, 2, 3 and 4 under two sigma levels i.e. 0.8 and 1.0. It was discovered that when the sample size is small (n = 20), UBR and GCV were equally preferred and for n = 60 and 100 at smoothing parameters (λ = 1, 2, 3 and 4) UBR method was the best for estimating the degree of smoothness.*

KEYWORDS*:Generalized Maximum Likelihood, Generalized Cross-Validation, Unbiased Risk, Proposed Smoothing Method, Predictive Mean Square Error, Splines Smoothing and Time series.*

Date of Submission: 10-07-2019 Date Of Acceptance: 28-07-2019

I. INTRODUCTION

Non parametric regression is a type of Regression analysis where the predictor does not take a predetermined form but relies on information collected from the observation. The nonparametric regression can be used to estimate a regression curve by providing a broad based method of exploring the relationship between two variables, it can also be used for predictions of observations yet to be made without reference to a fixed parametric model. It can provides a techniques for spurious observations by studying the influence of isolated points, it constitutes a flexible method of substituting missing values or interpolating between adjacent X-values. The general spline smoothing model is given as:

$$y_i = f\left(X_i\right) + \varepsilon_i \quad (1)$$

Where; y_i is the observation values of the response variable y, f is an unknown smoothing function, X_i is the observation values of the predictor variable x and ε_i is normally distributed random errors with zero mean and constant variance.

The main objective of this research is to estimate f (.) when $x_i = t_i$ but not necessarily equally spaced, with $t_1 < . . . < t_n$(time) and ε_i is assumed to be correlated. [6]. Therefore, this research shall consider the spline smoothing for non-parametric estimation of a regression function in a time-series context with the model;

$$y_i = f\left(t_i\right) + \varepsilon_{ti} \quad (2)$$

Where; y_i = observation values of the response variable y, f = an unknown smoothing function, t_i = time for i = 1 . . . n, ε_{ti} = zero mean autocorrelated stationary process.

Smoothing spline arises as the solution to a nonparametric regression problem having the function f(x) with two continuous derivatives that minimizes the penalized sum of squares

$$S(f) = \sum_{i-1}^{n}\left(y_i - f(x_i)\right)^2 + \lambda \int_0^1 \left(f^{II}(x)\right)^2 dx \quad (3)$$

Where; λ is the smoothing parameter, the first term in the equation is the residual sum of square, the second term is a roughness penalty, which is large when the integrated second derivative of regression function $f^{II}(x)$ is large when f(x) is rough (i.e. with rapidly changing slope). The parameter λ controls the trade-off between goodness-of-fit and the smoothness of the estimate and is often referred to as the smoothing parameter. If λ is 0 then f(x) simply interpolates the data, if λ is very large, then f(x)will be selected so that $f^{II}(x)$ is everywhere, which implies a globally linear least-squares fit to all data. There is the need to tackle the problem associated with estimating the best spline smoothing methods for time series observation when the error term is independently identically distributed.

There are vast literatures on Spline Smoothing modeling of correlational observations; [19], [10], [23], [18], [20], [3], [14], [4], [7], [9], [16], [8], [15], [21], [10], [13], [5], [2], [11] and [1].

This paper aim to propose a new smoothing method (PSM) by modifying two of the existing Spline Smoothing methods (i.e. the Generalized Cross Validation (GCV) and Unbiased Risk (UBR) and compare its efficiency and performance with three existing estimation methods namely; Generalized Maximum Likelihood (GML), Generalized Cross Validation (GCV) and Unbiased Risk (UBR). Spline smoothing estimation methods for time series observation were discussed in section one. Section two reviews the existing spline smoothing method and the proposed selection method, Section 3presents the Monte Carlo simulation study, equation used for generating values in simulation and experimental design and data generation, section four compares the four methods via a simulation study, and finally, the result discussion and conclusion were presented in last section.

II. ESTIMATION OF PARAMETERS

2.1 Generalized Cross-Validation (GCV) estimate method:

The term Generalized Cross-Validation (GCV) was coined by [16] and was applied by [22], [2]. The GCV score which is constructed by analogy to CV score can be obtained from the ordinary residuals by dividing by the factors$1-(S_\lambda)_{ii}$. The underlying design of GCV is to replace the factors $1-(S_\lambda)_{ii}$ in equation (4) with the average score$1-\frac{1}{n}\mathrm{tr}(S_\lambda)$. Thus, by summing the squared corrected residual and factor$\{1-\frac{1}{n}\mathrm{tr}(S_\lambda)\}^2$, based on the analogy of Ordinary Cross-Validation, the GCV score function can be written mathematically as;

$$\mathrm{GCV}(\lambda) = \frac{1}{n}\frac{\sum_{i=1}^{n}\{y_i-\hat{f}_\lambda(x_i)\}^2}{\{1-\frac{1}{n}\mathrm{Trace}\ (S_\lambda)\}^2} = \frac{\frac{1}{n}\|(I-S_\lambda)y\|^2}{\left[\frac{1}{n}\mathrm{trace}\ (I-S_\lambda)\right]^2} \quad (4)$$

Where; n is the pairs of measurement/observations $\{x_i,y_i\}$, λ is the Smoothing parameters and S_λ is the ith diagonal element of smoother matrix

2.2 Generalized Maximum Likelihood (GML) estimate method

A Bayesian model provides a general framework for the GML method and can be used to calculate the posterior confidence intervals of a spline estimate. It is defined as;

$$\mathrm{GLM}(\lambda) = \frac{y^I(I-S_\lambda)y}{[\det^+(I-S_\lambda)]^{\frac{1}{n-m}}} \quad (5)$$

Where; Det^+ is the product of the nonzero eigenvalues, y^I is the estimate of y is smoothing parameter, S_λ is the diagonal element of smoother matrix, n is the pairs of measurement/observations {xi,yi}and m is number of zero eigenvalues

2.3 Unbiased Risk (UBR) estimate method

The UBR method or CP criterion was suggested by [12] and had been applied successfully by Craven and [17],[24], [19]; [6] and [22] for selecting smoothing parameters for spline estimates with non-Gaussian data. It is written as;

$$\mathrm{UBR}(\lambda) = \frac{1}{n}\{\|(S_\lambda - 1)y\|^2 + 2\sigma^2\mathrm{tr}(S_\lambda) - \sigma^2\}$$

$$\mathrm{UBR}(\lambda) = \frac{1}{n}\left\{\left\|(y-\hat{f}_\lambda)y\right\|^2 + 2\sigma^2\mathrm{tr}(S_\lambda) - \sigma^2\right\}$$

$$\mathrm{UBR}(\lambda) = \frac{1}{n}\frac{\sum_{i=1}^{n}\{y_i-\hat{f}_{\hat{\lambda}}(x_i)\}^2}{\mathrm{tr}\{I-(S_{\hat{\lambda}})\}^2} = \frac{\|(S_{\hat{\lambda}}-I)y\|^2}{\mathrm{tr}(I-S_{\hat{\lambda}})} \quad (6)$$

Where; y is the Smoothing parameter, $S_{\hat{\lambda}}$is the ith diagonal element of smoother matrix, n is the pairs of measurement/observations $\{x_i,y_i\}$

2.4 Proposed Smoothing Method (PSM) with Autocorrelation Structure

$$\mathrm{PSM}(\lambda) = \frac{\|(I-S_\lambda)y\|^2}{\frac{1}{n}\mathrm{tr}(I-S_\lambda)\|(S_\lambda - I)y\|^2} \quad (7)$$

Where; n is Pairs of observation and $S_\lambda$is the diagonal element of smoother matri**x**

III. MATERIALS AND METHODS

A simulation study is conducted to evaluate and compare the performance of the four estimation methods presented in previous sections. The model considered is;

$$y(t) = \frac{\mathrm{Sin}\,\pi}{t} + \varepsilon_t \qquad t = 1, \ldots, 100 \qquad (8)$$

Where; ε's are generated with mean 0, standard deviations 0.8 and 1.0

A Monte Carlo simulation study was conducted to evaluate the performances of the four selection methods described in this study i.e. GML, GCV, UBR and PSM. Data were simulated by using a program coded in R (version 3.2.3) for smoothing functions λ = 1, 2, 3 and 4, sample sizes; 20, 60 and 100, two standard deviation were considered i.e. σ = 0.8 and 1.0. The number of replications was 1000 for each of the samples. For each simulated data sets, the predictive mean squared-errors (PMSE) were used to evaluate the quality of estimate, it is written mathematically as;

$$\mathrm{PMSE}(\lambda) = \mathrm{E}\left[\sum_{i=1}^{n}\left(f(x_i) - \hat{f}(x_i)\right)^2\right] \quad (9)$$

The Predictive Mean Square Error can be divided into two terms, the first term is the sum of square biases of the fitted values while the second is the sum of variances of the fitted values.

Where;

$f(x_i)$ = observed value and $\hat{f}(x_i)$= fitted/predicted/estimated value

$$\mathrm{PMSE}(\lambda) = \sum_{i=1}^{n}\left(\mathrm{E}\left[\hat{f}(x_i)\right] - f(x_i)\right)^2 = \sum_{i=1}^{n}\mathrm{var}\left[\hat{f}(x_i)\right] \quad (10)$$

IV. SIMULATION RESULT

In this study, a modified Spline smoothing estimation method and compared its efficiency with three existing estimation methods namely; the Generalized Cross-Validation, Generalized Maximum Likelihood and Unbiased Risks, we computed Predictive mean square errors criterion to measure their efficiency.

Table 4.1: PMSE result for the smoothing methods when there is no autocorrelation for smoothing parameters (λ = 1, 2, 3 and 4), time (T = 20, 60 and 100) and std. deviation (σ = 0.8)

Time size	Smoothing Methods	Smoothing Parameter levels			
		λ = 1	λ = 2	λ = 3	λ = 4
T =20	GCV	0.053273	0.044131	0.042976	0.042599
	GML	0.081617	0.082523	0.082663	0.082711
	PSM(k=1)	100.4239	82.71148	79.70962	78.68089
	UBR	0.04802	0.032269	0.030172	0.017179
T = 60	GCV	0.027264	0.021027	0.020245	0.029484
	GML	0.074695	0.07129	0.070683	0.070472
	PSM(k=1)	38.44716	31.91883	30.81778	30.44087
	UBR	0.034561	0.024042	0.022625	0.022158
T = 100	GCV	0.025094	0.018843	0.018061	0.017806
	GML	0.068976	0.067162	0.066835	0.066721
	PSM(k=1)	4.003851	3.198199	3.069462	3.02584
	UBR	0.025485	0.018456	0.017496	0.017179

The table above presents the predictive mean square error for the four estimators, three time periods, and four spline smoothing levels at 0.8 sigma level. It was discovered that for GCV;the predictive mean square error decreases from 0.053273 to 0.027264 to 0.025094 as the time series sample increases from T = 20 to 60 and to 100 for λ =1. For GML; the predictive mean square error decreases from 0.082663 to 0.070683 and then to 0.066835 as the time series sample increases from T = 20 to 60 and to 100 for λ =3. For PSM;the predictive mean square error decreases from 78.68089 to 30.44087 and then to 3.02584 as the time series sample increases from T = 20 to 60 and to 100 for λ =4 and for UBR, the predictive mean square error decreases from 0.030172 to 0.022625 and then to 0.017496 as the time series sample increases from T = 20 to 60 and to 100 for λ = 3.

Table 4.2: PMSE result for the smoothing methods when there is no autocorrelation for smoothing parameters (λ = 1, 2, 3 and 4), time (T = 20, 60 and 100) and std. deviation (σ = 1.0)

Time size	Smoothing Methods	Smoothing Parameter levels			
		λ = 1	λ = 2	λ = 3	λ = 4
T =20	GCV	0.1268264	0.104707	0.101912	0.101001
	GML	0.182682	0.18376	0.183906	0.183954
	PSM(k=1)	80.87162	62.52266	59.62848	58.65031
	UBR	0.056372	0.03999	0.037767	0.037034
T = 60	GCV	0.0424942	0.033899	0.032822	0.032471
	GML	0.0902741	0.087698	0.087233	0.087072
	PSM(k=1)	31.6832	24.93528	23.85243	23.48527
	UBR	0.0444551	0.030348	0.02846	0.027839
T = 100	GCV	0.0242396	0.019535	0.018947	0.018755
	GML	0.0598298	0.057675	0.05729	0.057156

PSM(k=1)	3.704103	2.900917	2.77374	2.730723
UBR	0.0373787	0.025315	0.023706	0.023177

Table 4.2 presents the predictive mean square error for the four estimators, three time periods, and four spline smoothing levels at 1.0 sigma level. It was discovered that for GCV;the predictive mean square error decreases from 0.104707 to 0.033899 to 0.019535 as the time series sample increases from T = 20 to 60 and to 100 for λ = 2. For GML;the predictive mean square error decreases from 0.183954 to 0.087072 and then to 0.057156 as the time series sample increases from T = 20 to 60 and to 100 for λ = 4. For PSM;the predictive mean square error decreases from 80.87162 to 31.6832 and then to 3.704103 as the time series sample increases from T = 20 to 60 and to 100 for λ = 1 and for UBR, the predictive mean square error decreases from 0.056372 to 0.0444551 and then to 0.0373787 as the time series sample increases from T = 20 to 60 and to 100 for λ = 1

4.3 Smoothing curves of the time series observation in the absence of Autocorrelation error

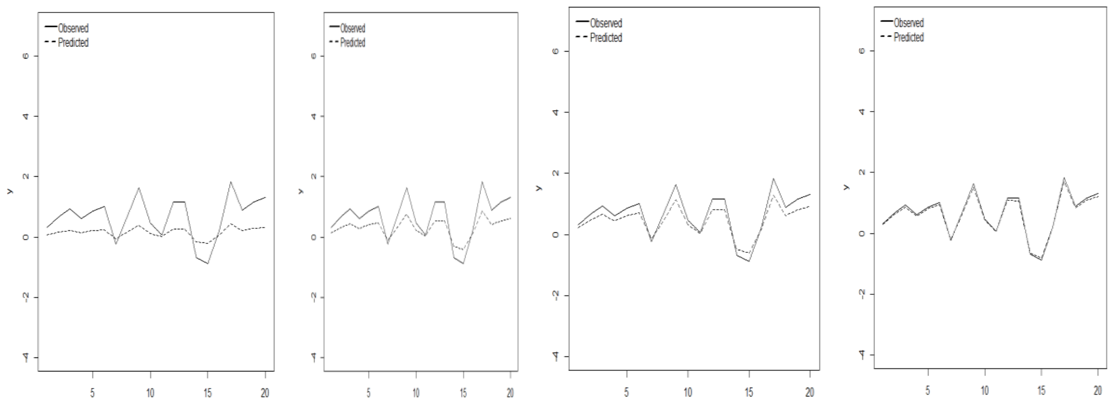

Figure 4.3.1: Plots of the observations (. . .) and Estimates (---) With Smoothing Parameters Chosen by GCV (a), GML (b), PSM (c), and UBR (d) for λ=1,2,3,4 σ = 0.8 and T = 20

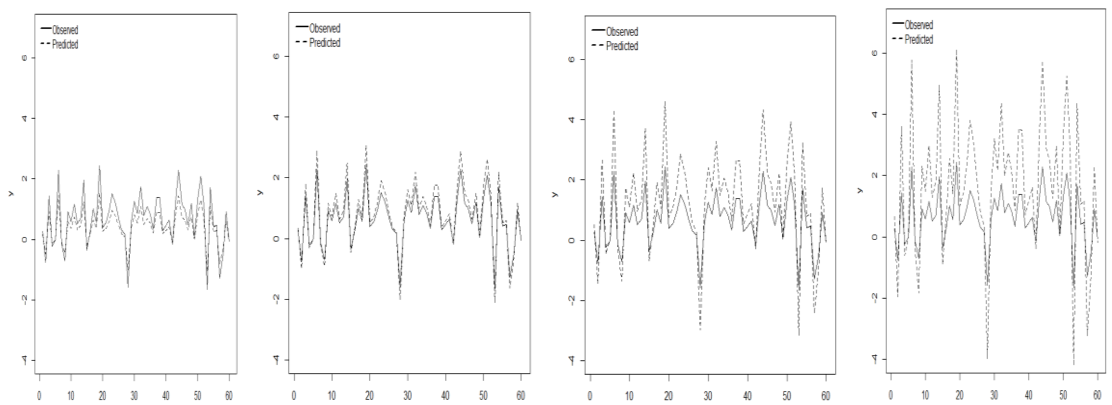

Figure 4.3.2: Plots of the observations (. . .) and Estimates (---) With Smoothing Parameters Chosen by GCV (a), GML (b), PSM (c), and UBR (d) for λ=1,2,3,4 σ = 0.8 and T = 60

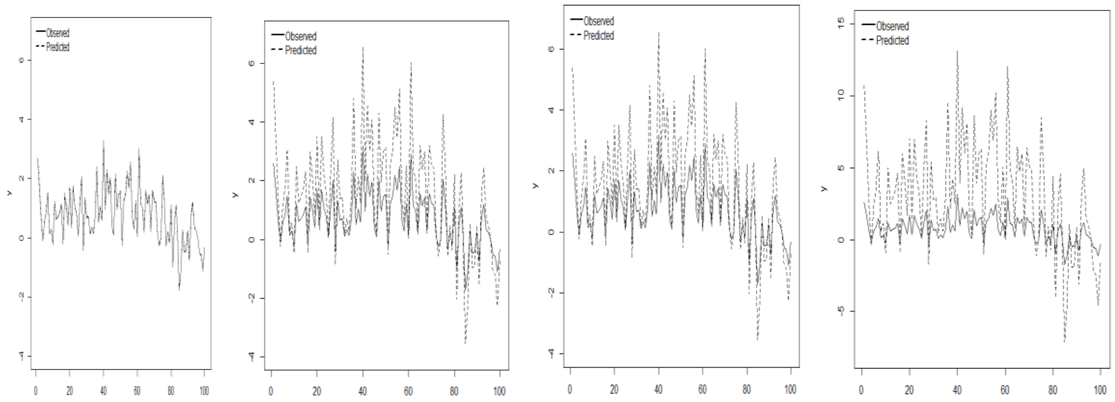

Figure 4.3.3: Plots of the observations (. . .) and Estimates (---) With Smoothing Parameters Chosen by GCV (a), GML (b), PSM (c), and UBR (d) for λ=1,2,3,4 σ = 0.8 and T = 100

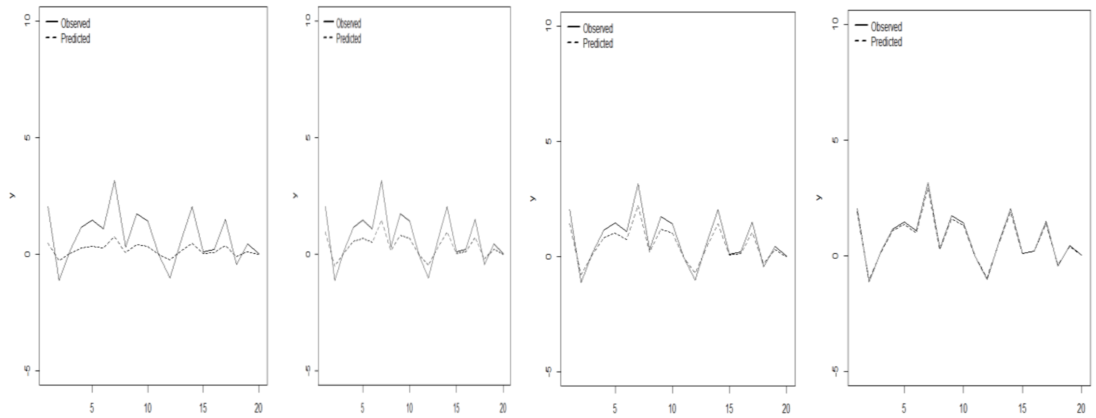

Figure 4.3.4: Plots of the observations (. . .) and Estimates (---) With Smoothing Parameters Chosen by GCV (a), GML (b), PSM (c), and UBR (d) for λ=1,2,3,4 σ = 1.0 and T = 20

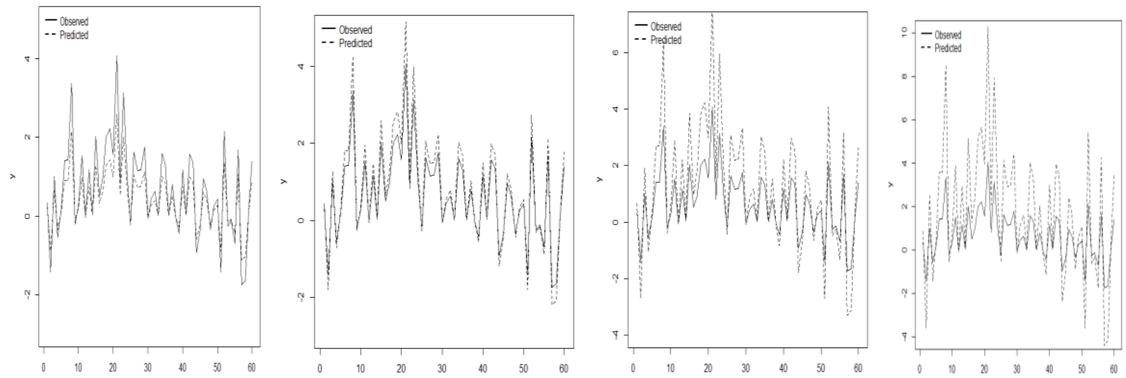

Figure 4.3.5: Plots of the observations (. . .) and Estimates (---) With Smoothing Parameters Chosen by GCV (a), GML (b), PSM (c), and UBR (d) for λ=1,2,3,4 σ = 1.0 and T = 60

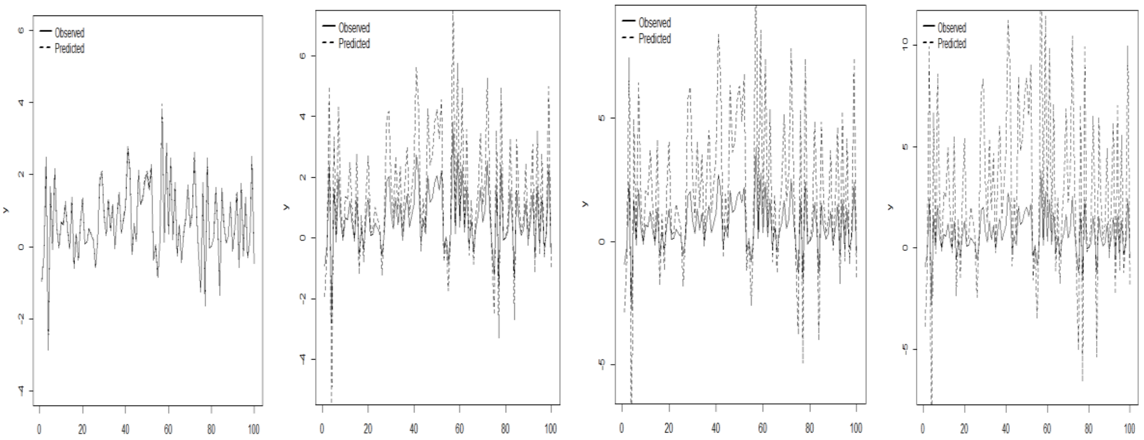

Figure 4.3.6: Plots of the observations (. . .) and Estimates (---) With Smoothing Parameters Chosen by GCV (a), GML (b), PSM (c), and UBR (d) for λ=1,2,3,4 σ = 1.0 and T = 100

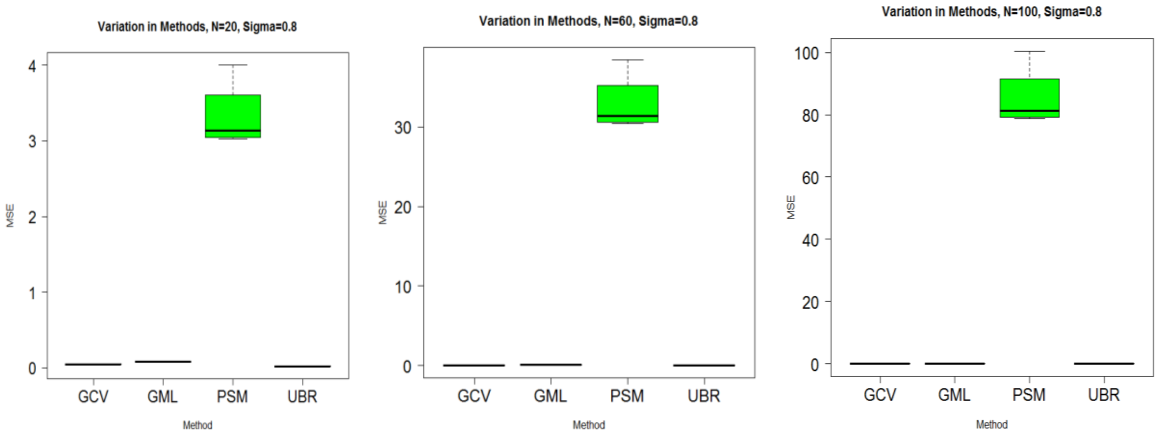

Figure 4.3.7: Box plot of the GML, GCV, PSM and UBR of the PMSE of the simulated study in the absence of autocorrelation when σ = 0.8 and T = 20, 60 and 100

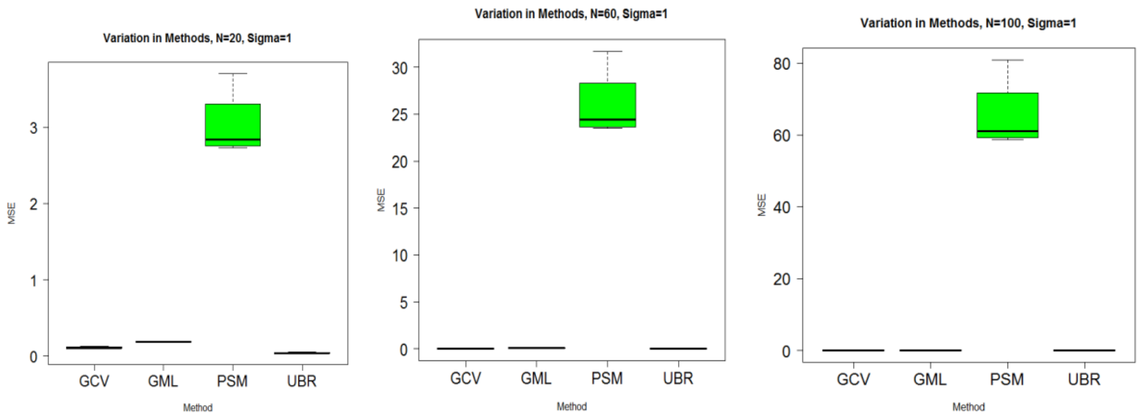

Figure 4.3.8: Box plot of the GML, GCV, PSM and UBR of the PMSE of the simulated study in the absence of autocorrelation when σ = 1.0 and T = 20, 60 and 100

Figures 4.3.1 – 4.3.8 above presents the plots of the estimates for GCV, GML, PSM and UBR for 1,000 replications in the absence of autocorrelation error based on the predictive mean square error criterion. From these plots it is observed that GCV, GML and UBR estimates has small Predictive mean square error compare to PSM. The GCV have a smaller PSME, but the PSM estimates have larger PSME. From the predictive mean-square errors and plots of the estimated functions (shown above) it is concluded that all three smoothing methods estimate the smoothing parameters and the functions well. The UBR and GCV provide better estimates than GML and PSM in terms of the predictive mean-square error. The UBR method is more stable when the sample size is small and moderate, such as when T = 20 and 60. In this case there were several replications where GML and PSM provided very small estimates of smoothing parameters which lead to over-fitting the data. This behavior of the method was investigated in Wahba and Wang (1993) and Wang (1998). The GCV method performs as well as the UBR method for large sample sizes (T = 100) and better than the GML and PSM method at all sample sizes. The UBR method is computationally more efficient than the GCV, GML and PSM methods. Overall the UBR method works well and is recommended for the time series observations in the absence of autocorrelation error.

Table 4.3A: Rank of the performance of smoothing methods when there is no autocorrelation for time periods = 20, 60 and 100, smoothing function = 1, 2, 3 and 4 and for std. dev. = 0.8

Time size	Smoothing Method	Smoothing Parameter levels			
		λ = 1	λ = 2	λ = 3	λ = 4
T =20	GCV	2	2	2	2
	GML	3	3	3	3
	PSM(k=1)	4	4	4	4
	UBR	1	1	1	1
T = 60	GCV	1	1	1	2
	GML	3	3	3	3
	PSM(k=1)	4	4	4	4
	UBR	2	2	2	1
T = 100	GCV	1	2	2	2
	GML	3	3	3	3
	PSM(k=1)	4	4	4	4
	UBR	2	1	1	1

Table 4.3B: Preferred smoothing methods at λ = 1, 2, 3 and 4 for time periods= 20, 60 and 100 and standard deviation = 0.8

Time series level	Smoothing Parameters			
	λ = 1	λ = 2	λ = 3	λ = 4
T = 20,	UBR	UBR	UBR	UBR
T = 60	GCV	GCV	GCV	UBR
T = 100	GCV	UBR	UBR	UBR

Table 4.3C: Rank of the performance of smoothing methods when there is no autocorrelation for time periods = 20, 60 and 100, smoothing function = 1, 2, 3 and 4 and for std. dev. = 1.0

Time size	Smoothing Method	Smoothing Parameter levels			
		λ = 1	λ = 2	λ = 3	λ = 4
T =20	GCV	2	2	2	2
	GML	3	3	3	3
	PSM(k=1)	4	4	4	4
	UBR	1	1	1	1
T = 60	GCV	1	2	2	2
	GML	3	3	3	3
	PSM(k=1)	4	4	4	4
	UBR	2	1	1	1
T = 100	GCV	1	1	1	1
	GML	3	3	3	3
	PSM(k=1)	4	4	4	4
	UBR	2	2	2	2

Table 4.3D: Preferred smoothing methods at λ = 1, 2, 3 and 4 for time periods= 20, 60 and 100 and standard deviation = 1.0

Time series level	Smoothing Parameters			
	λ = 1	λ = 2	λ = 3	λ = 4
T = 20,	UBR	UBR	UBR	UBR
T = 60	GCV	UBR	UBR	UBR
T = 100	GCV	GCV	GCV	GCV

V. DISCUSSION OF FINDINGS AND CONCLUSION

The four tables above presents ranks and preferred smoothing methods of the four smoothing methods/estimators (GCV, GML, PSM and UBR) of the four smoothing parameters (λ = 1, 2, 3 and 4) at three time periods (i.e. T = 20, 60 and 100) when the standard deviation is 0.8 and 1 in the absence of Autocorrelation error.

From the results present in table 4.3B, it can be seen that UBR estimator had the least predictive mean square error when the time series size is small (T = 20), GCV estimator had the smallest predictive mean square error when the time series size is moderate (T = 60) except when the smoothing parameter is four ($\lambda = 4$) and UBR estimator had the smallest predictive mean square error when the time series size is high (T = 100) except when the smoothing parameter is one ($\lambda = 1$).

From the results present in table 4.3C, it can be seen that UBR estimator had the least predictive mean square error when the time series size is small (T = 20), UBR estimator also had the smallest predictive mean square error when the time series size is moderate (T = 60) except when the smoothing parameter is one ($\lambda = 1$) and GCV estimator had the smallest predictive mean square error when the time series size is high (T = 100) at all levels of smoothing parameters.

In summary, UBR and GCV were the best estimators for time series observations in the absence of Autocorrelation at the four smoothing parameters (λ = 1, 2, 3 and 4), three time periods (i.e. T = 20, 60 and 100), for standard deviation (σ = 0.8 and 1) based on the predictive mean square error (PSME) criterion.

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Samuel Olorunfemi Adams" A Proposed Spline Smoothing Estimation Method for Time Series Observations"International Journal of Mathematics and Statistics Invention (IJMSI), vol. 07, no. 02, 2019, pp.18-25